

An Investigation into Chemical Kinetics and the Arrhenius Equation for Activation Energy

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INTRODUCTION

The idea for this investigation came about when I was trying to open a bottle of soda. It had been tossed around inside my bag, so it fused up when I tried to open it. A friend of mine told me that if I opened it slowly, the foam would be released over a longer period, leading to less spilling. This led me to investigate something regarding rate. After learning about the rate of reaction in class, I decided that I wanted to investigate the relationship between temperature and rate. But why might this be a relevant field of investigation in the scientific community? Fritz Haber discovered by looking at rates that the speed of the reaction depended largely on the fact that the triple bond in nitrogen is really hard to break. He and his assistant were able to develop catalysts which allowed this process to occur at a much faster rate. ¹ This developed into the Haber process, which is used to produce fertilizer today, almost 100 years after its discovery. ²

The mathematical model for the Haber process was developed by a Swedish scientist named Arrhenius. He was both a physicist and chemist, and his work is closely linked to the Maxwell-Boltzmann energy distribution for different temperatures (Figure 1 ³). This is what we call collision theory which states that with a higher temperature, the number of molecules that have kinetic energy above the activation energy, will be greater. This should in theory make the reaction proceed faster, meaning that the rate would be greater. In this investigation, I wish to look at the relationship between initial rate and temperature, as well as experimentally determine the Arrhenius Activation energy (E_a) for the reaction between sodium carbonate and dilute hydrochloric acid.

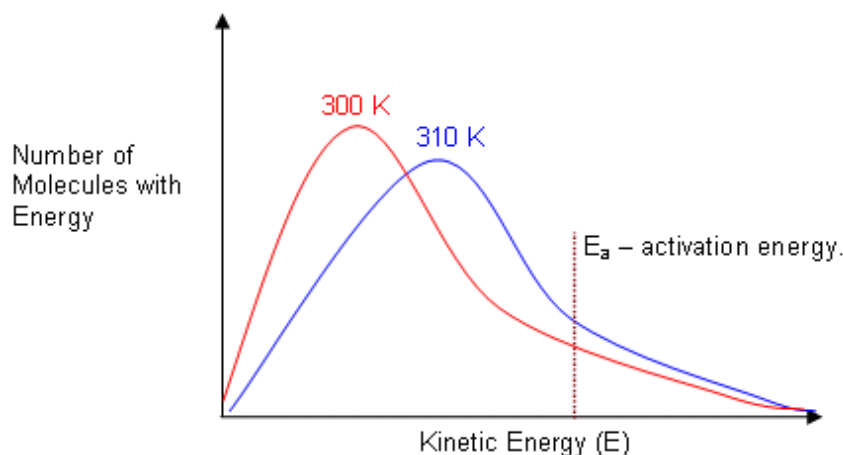
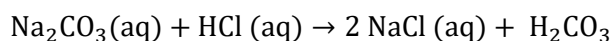
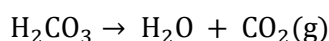


Figure 1. Maxwell - Boltzmann energy distribution.

In order to test the effect of temperature on the initial rate of reaction, I found a chemical reaction that produces a gas to measure the rate at which the gas is produced. Sodium carbonate reacts with hydrochloric acid, carbonic acid is produced.



Since carbonic acid is unstable, it decomposes as shown in the reaction below:

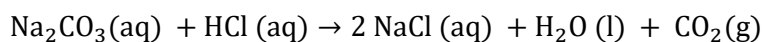


¹ "Chemistry - Rates of Reaction," *University of Birmingham*, last modified 2020, accessed January 27, 2021, <https://www.birmingham.ac.uk/teachers/study-resources/stem/chemistry/reaction-rates.aspx>.

² Wikipedia Contributors, "Haber Process," *Wikipedia* (Wikimedia Foundation, January 20, 2021), last modified January 20, 2021, accessed January 28, 2021, https://en.wikipedia.org/wiki/Haber_process.

³ Horrocks, Mathew. "Reaction Rates, Temperature and Catalysis." *4college.Co.Uk*. Last modified 2020. Accessed October 24, 2020. <http://www.4college.co.uk/a/aa/rate.php>.

The final reaction will therefore be:



Hence, we can measure the rate at which carbon dioxide gas is produced. This would allow us to calculate the initial rate, as well as calculating the activation energy for this reaction.

$$k = Ae^{-\frac{E_a}{RT}} \quad \text{or} \quad \ln k = -\frac{E_a}{RT} + \ln A$$

Where:

k	=	Chemical Reaction Rate
A	=	Pre-exponential Factor
E_a	=	Activation Energy
R	=	Gas Constant
T	=	Temperature in Kelvin

Figure 2. Linearization of Arrhenius Equation.

To find the activation energy, I first need to find the rate constant. As seen in Figure 2⁴, if I plot the natural logarithm of the rate constant on the y-axis, and $\frac{1}{T}$ on the x-axis, the gradient of the graph will be $-\frac{E_a}{R}$ where R is the gas constant. This means that the activation energy is the gradient multiplied by -8.31. The rate constant can be calculated from the rate law. The rate law in its power form is as follows:

$$\text{rate} = k * [\text{A}]^n * [\text{B}]^m$$

Where k is the rate constant, $[\text{A}]$ and $[\text{B}]$ are the concentration of reactants, and n and m are rate orders. The law of mass action predicts that a reaction in a dilute solution, the rate only depends on the concentration of the reactants, raised to the power of their stoichiometric coefficients.⁵ Since the concentration of sodium carbonate is 1.0, the rate order n does not matter. The stoichiometric coefficient for hydrochloric acid is 2, and its molarity is 2.0. Hence, the rate constant is given by the following equation:

$$k = \frac{\text{Initial rate}}{2.0^2} = \frac{\text{Initial rate}}{4}$$

Research questions: What is the relationship between temperature and initial rate? What is the activation energy for the reaction between sodium carbonate and hydrochloric acid?

Independent variable: Temperature

Dependent variable: Rate of reaction

Research hypothesis: The initial rate of reaction will be greater at higher temperatures.

⁴ "Arrhenius Equation and Stability Studies," *Blogspot.com*, last modified 2012, accessed January 29, 2021, <http://stabilitystudies.blogspot.com/2012/06/arrhenius-equation-and-stability.html>.

⁵ "Physical Chemistry," *Google Books*, last modified 2013, accessed January 27, 2021, https://books.google.no/books?id=lk2PzH9Lms8C&dq=isbn:0716787598&hl=no&sa=X&ved=2ahUKEwiYz_S8wr_uAhVuAhAIHZerDMgQ6AEwAHoECAAQAg.

EQUIPMENT AND CHEMICALS

Equipment

- Digital scale $\pm .001$ g
- Thermometer $\pm .05$ °C
- 2x Pipette 10.000 ml $\pm .020$ ml
- 3x Beaker 100 ml
- Beaker 300 ml ± 5 ml (for solution)
- Beaker >400ml (for waste)
- 2x Vertically standing arms
- Clamp
- Erlenmeyer flask 50 ml
- Rubber bung (sized to fit the Erlenmeyer flask)
- Small tube
- Graduated measuring cylinder 50.00 ml ± 0.05 ml
- Suitable clamp for the measuring cylinder
- Wide jar to create water trough
- Video capturing device
- Water bath
- Magnetic stirrer

Chemicals

- Sodium carbonate, Na_2CO_3 (s). Dissolved in water to make a solution with 1.00 ± 0.08 mol dm^{-3} .
- Dilute hydrochloric acid, HCl (aq), 2.0 ± 0.1 mol dm^{-3} .

METHOD

Risk assessment

Sodium carbonate, Na_2CO_3 , is a base and causes serious irritation if it comes in contact with the eyes. To account for this, I wore glasses and I avoided touching my face when handling the chemicals.

Hydrochloric acid, HCl , is a strong acid and can cause skin corrosion and irritation. To prevent this, I made sure that the acid only persisted in the beaker in which it was heated and cooled in, as well as in the pipette. I also washed my hands after handling the acid.

The chemicals were not heated directly but rather placed into separate beakers that were placed into the water bath. The water bath was not heated with a hotplate for other trials than the one with the highest temperature, and the lower temperatures were rather placed into hot tap water. The fridge used to cool the solutions was a fridge designated to the lab, only containing chemicals and no food.

Once all trials for all temperatures were complete, the beaker with sodium chloride was emptied into a suitable container for chemical waste.

Procedure

Step 1: Initial setup and preparation of chemicals

I started by setting up the equipment as shown in Figure 3. The main takeaways are that the Erlenmeyer flask has to be higher in elevation than the bottom measuring cylinder which collects the gas. This is so that the gas will flow from the flask and into the measuring cylinder, displacing the water already in it. By doing this, I was able to read the volume of carbon dioxide gas, which equals the volume of water being displaced.

When I was preparing the sodium carbonate solution, I performed several test trials to deduce which concentration was suitable for my experiment. This was done to make sure that the rate of the reaction would be neither too big nor too small. The results of my test trials were that 1.00 mol dm^{-3} sodium carbonate was suitable. In the 300 ml beaker, I prepared 300 ml of solution (an excess amount of what I needed). This was done by measuring $31.821 \text{ g} \pm 0.001 \text{ g}$ sodium carbonate ($M_r(\text{Na}_2\text{CO}_3) * 0.3$) and dissolving it in $300 \text{ ml} \pm 5 \text{ ml}$ of water. I used a magnetic stirrer to make sure it dissolved fully in the water. By the stoichiometric relation between sodium carbonate and hydrochloric acid, 1:2, I decided to use 2.0 mol dm^{-3} of HCl.

Step 2: Achieving the desired temperatures

Around 50 ml of sodium carbonate solution and hydrochloric acid were poured into separate 100 ml beakers. These beakers were placed in the fridge for the coldest temperature, left at room temperature for the second temperature, and for the three hottest trials they were heated in the same water bath. I measured the temperature of the sodium carbonate. I assume that the temperature is the same for HCl. When the desired temperature was reached, the beakers were removed from the water bath.

Step 3: Mixing the reactants

After removing the beakers from the water bath, I immediately recorded the temperature of the sodium carbonate. I used one of the $10.000 \text{ ml} \pm .020 \text{ ml}$ pipettes and measured $10.000 \text{ ml} \pm .020 \text{ ml}$ sodium carbonate and emptied the pipette into the Erlenmeyer flask. Then I took the other $10.000 \text{ ml} \pm .020 \text{ ml}$ pipette and measured $10.000 \text{ ml} \pm .020 \text{ ml}$ of hydrochloric acid. When performing my test trials, I initially took the HCl from the pipette directly into the Erlenmeyer flask, but when the pipette was empty, and I was going to place the rubber bung, the rate at which the bubbles were forming had already decreased a lot. Hence, the acid was placed into a beaker in order to pour it into the Erlenmeyer flask quicker. I continued by pouring the acid into the flask as quickly as I could without spilling. The rubber bung was placed into the opening of the Erlenmeyer flask immediately after while making sure the seal was tight. I waited 30 seconds for the reaction to take place and then ended the trial.

Step 4: Measuring the volume of gas

The production of gas and displacement of water was recorded with the camera on my phone for each trial. The volume of carbon dioxide gas was read off by looking at the videos and noting down how much water was displaced after time intervals of 3 seconds. The products left in the Erlenmeyer flask was poured into a separate waste beaker with a volume of 600 ml. Steps 2 through 4 were repeated three times for 5 different temperatures: $T_1=10^\circ\text{C}$, $T_2=22^\circ\text{C}$, $T_3=30^\circ\text{C}$, $T_4=40^\circ\text{C}$, and $T_5=50^\circ\text{C}$.



Figure 3. Setup of the experiment. Water bath not shown.

RAW DATA

Table 1. Raw data from temperature 3. T_0 is the initial temperature. All the volumes in Table 1 are the volume of CO_2 gas (displaced water) after X seconds.

Temperature 3	Trial 1	Trial 2	Trial 3
T_0 in $^{\circ}\text{C}$ ($\pm .05$ $^{\circ}\text{C}$)	31.00	31.80	30.10
3s ($\pm .05$ ml)	3.60	3.70	3.20
6s ($\pm .05$ ml)	9.10	8.50	5.40
9s ($\pm .05$ ml)	9.60	9.30	6.10
12s ($\pm .05$ ml)	10.20	10.00	7.10
15s ($\pm .05$ ml)	10.90	10.50	7.85
18s ($\pm .05$ ml)	11.40	11.45	8.30
21s ($\pm .05$ ml)	12.00	12.15	8.70
24s ($\pm .05$ ml)	12.35	12.85	9.70
27s ($\pm .05$ ml)	13.00	13.30	10.40
30s ($\pm .05$ ml)	13.45	14.10	11.00

The data set is very spacious (5x3x11). Therefore, to save space, I have only included the raw data for temperature 3 (Table 1). The rest can be found in Appendix A. I will use the data from the three trials with temperature 3 to show my work in calculating the initial rate and the activation energy.

A qualitative observation was when the reaction proceeded, bubbles were produced. This was the carbon dioxide that I attempted to collect. A fizzling sound was also produced together with the bubbles.

PROCESSED DATA

Calculating initial rate

To calculate the initial rate for each temperature, I calculated the average initial temperature as well as the average volume of gas collected after X seconds.

Table 2. Average values for the five temperatures. The uncertainties stated are from the equipment.

	T_1	T_2	T_3	T_4	T_5
T_0 in $^{\circ}\text{C}$ ($\pm .05$ $^{\circ}\text{C}$)	14.13	21.40	30.97	37.80	51.17
3s ($\pm .05$ ml)	0.00	0.00	0.00	0.00	0.00
6s ($\pm .05$ ml)	5.50	1.02	3.50	3.35	3.33
9s ($\pm .05$ ml)	8.73	3.92	7.70	5.85	11.78
12s ($\pm .05$ ml)	9.68	4.95	8.30	6.22	12.40
15s ($\pm .05$ ml)	10.42	5.53	9.10	6.5	12.77
18s ($\pm .05$ ml)	10.98	6.03	9.80	6.52	13.07
21s ($\pm .05$ ml)	11.60	6.68	10.40	6.67	13.43
24s ($\pm .05$ ml)	12.08	7.30	11.00	6.88	13.77
27s ($\pm .05$ ml)	12.68	7.65	11.60	7.00	13.98
30s ($\pm .05$ ml)	13.40	8.10	12.20	7.15	14.20

Data calculations

I made a table in Logger Pro using both manual and calculated columns, so I only had to plot in a couple of values, instead of all. This made it easier to process the large data set since it involves a fair number of calculations per temperature. The number of moles of CO₂ is calculated from the ideal gas law.

$$pV = nRT$$

$$n = \frac{pV}{RT}$$

Where p is pressure in Pascal, V is the volume in m³, n is the number of moles, R is the gas constant and T is the temperature in Kelvin. In my case, V is the volume of CO₂ and temperature is the initial temperature in Kelvin. I have to assume that the pressure in the measuring cylinder follows STP conditions (100kPa). In the calculations, I have made sure to change the units to fit the equation. The following shows the calculation for row 2 in Table 3 (page 8, time = 3 seconds).

$$n(\text{CO}_2 \text{ produced}) = \frac{pV}{RT} = \frac{10^5 * 3.50 * 10^{-6}}{8.31 * (30.97 + 273)} = .000139 \text{ mol (3 s. f.)}$$

$$c(\text{Na}_2\text{CO}_3) = \frac{n(\text{Na}_2\text{CO}_3 \text{ remaining})}{V(\text{Na}_2\text{CO}_3)} = \frac{(n(\text{Na}_2\text{CO}_3 \text{ initial}) - n(\text{CO}_2 \text{ produced}))}{V(\text{Na}_2\text{CO}_3 \text{ used})}$$

$$\begin{aligned} n(\text{Na}_2\text{CO}_3 \text{ remaining}) &= n(\text{Na}_2\text{CO}_3 \text{ initial}) - n(\text{CO}_2 \text{ produced}) \\ &= (1.0 \text{ mol dm}^{-3} * 10.0 \text{ ml} * 10^{-3}) - .000139 = .010 - .000139 \\ &= .00986 \text{ (3. s. f.)} \end{aligned}$$

This value is stated more accurately than it should. Rounding off all the values mid-calculation would not yield a good result. Hence, I choose to keep the number of moles with three significant figures, and not round off anything except the Activation Energy at the end.

$$\text{Concentration after 3s} = \frac{1.0 - .000139}{0.010} = .986 \text{ mol dm}^{-3}$$

Uncertainty calculations

$$\% \text{ uncertainty in temperature} = \frac{\text{measurement uncertainty}}{\text{measured temperature}} * 100 = \frac{.05}{30.97} * 100 = .16\% \text{ (2 s. f.)}$$

$$\% \text{ uncertainty in volume} = \frac{\text{measuring uncertainty}}{\text{measured volume}} * 100 = \frac{.05}{3.50} * 100 = 1.4\% \text{ (2 s. f.)}$$

$$\begin{aligned} \text{Abs. uncertainty } n(\text{CO}_2) &= \frac{(\% \text{ uncertainty in temperature} + \% \text{ uncertainty in volume})}{100} * n(\text{CO}_2) \\ &= \frac{(.16\% + 1.4\%)}{100} * .000139 = \pm 2.2 * 10^{-6} \text{ mol (2 s. f.)} \end{aligned}$$

$$\% \text{ Uncertainty } n(\text{Na}_2\text{CO}_3 \text{ initial}) = \left(\frac{.001}{31.821} + \frac{5.0}{300} + \frac{.020}{10.0} \right) * 100 = 1.9\% \text{ (2 s. f.)}$$

$$\text{Abs. uncertainty } n(\text{Na}_2\text{CO}_3 \text{ initial}) = \frac{1.9}{100} * (1.0 * 10 * 10^{-3}) = \pm 1.9 * 10^{-4} \text{ mol (2 s. f.)}$$

$$\begin{aligned} \% \text{ Uncertainty } n(\text{Na}_2\text{CO}_3 \text{ remaining}) &= \frac{(\text{Abs. uncertainty } n(\text{Na}_2\text{CO}_3 \text{ initial}) + \text{abs. uncertainty } n(\text{CO}_2))}{n(\text{Na}_2\text{CO}_3 \text{ remaining})} * 100 \\ &= \frac{(1.9 * 10^{-4} + 2.2 * 10^{-6})}{.00986} * 100 = 1.9\% \text{ (2 s. f.)} \end{aligned}$$

$$\% \text{ Uncertainty in } v(\text{Na}_2\text{CO}_3 \text{ used}) = \frac{.020}{10.0} * 100 = .20\% \text{ (2 s. f.)}$$

$$\% \text{ Uncertainty in concentration} = 1.9\% + .20\% = 2.1\% \text{ (1 d. p.)}$$

$$\text{Abs. uncertainty in concentration} = \frac{2.1\%}{100} * 0.986 = \pm .021 \text{ (2 s. f.)}$$

Table 3. Processed data for T₃. Data from Table 2. The columns containing delta (Δ) shows uncertainty with either percentage or absolute values (as stated in the parentheses). These are needed since the uncertainty in equipment will affect the calculations later. All uncertainties are rounded to two significant figures. ⁶

		Temperature 3										
	Time (s)	Temp. (°C)	ΔT (%)	V(CO ₂) (ml)	ΔV (%)	n(CO ₂) (mol)	Δn (CO ₂) (Absolute)	Na ₂ CO ₃ remaining (mol)	$\Delta \text{Na}_2\text{CO}_3$ (%)	[Na ₂ CO ₃] (mol dm ⁻³)	$\Delta [\text{Na}_2\text{CO}_3]$ (%)	$\Delta [\text{Na}_2\text{CO}_3]$ (Absolute)
1	0,0	30,97	0,16	0,00		0,00000		1,00E-02		1,0		
2	3,0	30,97	0,16	3,50	1,4	0,00014	2,2E-06	9,86E-03	1,9	0,99	2,1	0,021
3	6,0	30,97	0,16	7,70	0,65	0,00030	2,5E-06	9,70E-03	2,0	0,97	2,2	0,021
4	9,0	30,97	0,16	8,30	0,60	0,00033	2,5E-06	9,67E-03	2,0	0,97	2,2	0,021
5	12,0	30,97	0,16	9,10	0,55	0,00036	2,6E-06	9,64E-03	2,0	0,96	2,2	0,021
6	15,0	30,97	0,16	9,80	0,51	0,00039	2,6E-06	9,61E-03	2,0	0,96	2,2	0,021
7	18,0	30,97	0,16	10,40	0,48	0,00041	2,6E-06	9,59E-03	2,0	0,96	2,2	0,021
8	21,0	30,97	0,16	11,00	0,45	0,00044	2,7E-06	9,56E-03	2,0	0,96	2,2	0,021
9	24,0	30,97	0,16	11,60	0,43	0,00046	2,7E-06	9,54E-03	2,0	0,95	2,2	0,021
10	27,0	30,97	0,16	12,20	0,41	0,00048	2,8E-06	9,52E-03	2,0	0,95	2,2	0,021
11	30,0	30,97	0,16	12,90	0,39	0,00051	2,8E-06	9,49E-03	2,0	0,95	2,2	0,021

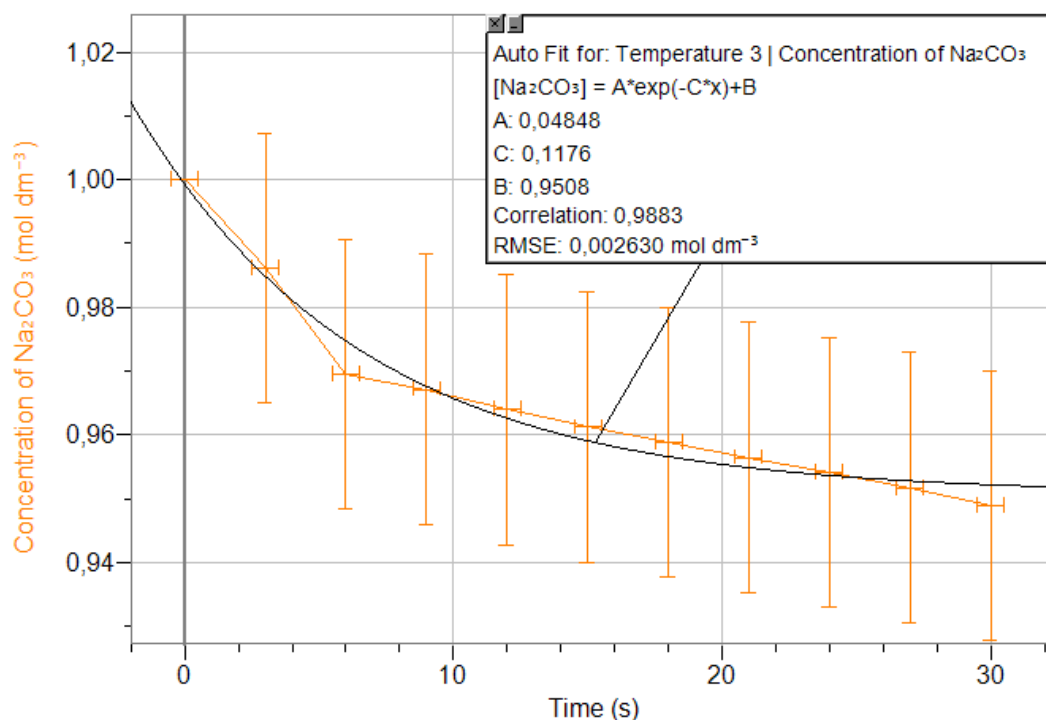


Figure 4. The regression line for data in Table 4, plotting a concentration-time graph for Temperature 3.

The initial rate is given by the rate of change of concentration when time = 0s, which means a tangent to the graph in Figure 4 at t=0s. I plotted the values from the regression line on a graphing calculator and found the initial rate (Figure 6). This process was repeated for all five temperatures and the results can be found in Table 4.

⁶ Similar tables for T₁ through T₅ is located in Appendix B.

For T_2 through T_5 the initial rate is increasing when the temperature is higher. This is visualized in Figure 5, which shows a general increase with higher temperatures. This is not the case for T_1 . Since T_1 is an outlier it will be discarded for the rest of the calculations. I will discuss this in the evaluation part of the paper.

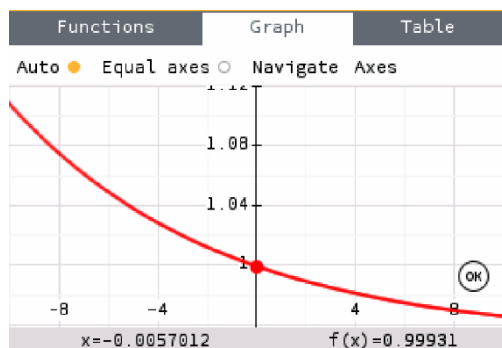


Figure 6. Initial rate for Temperature 3. ($dy/dx = -0.0057012$)

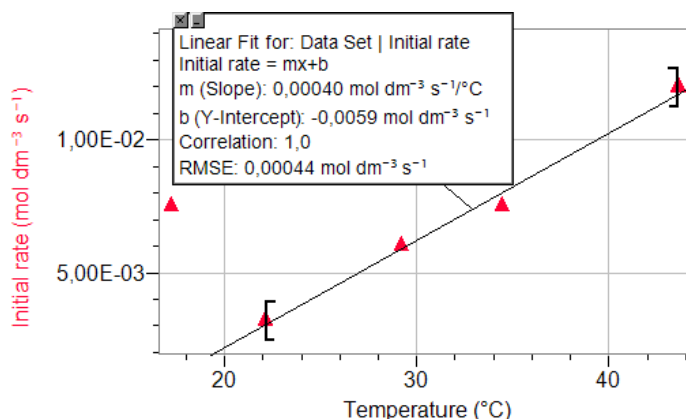


Figure 5. Initial rate and temperatures. Best-fit line without T_1 .

Calculating the activation energy

Table 4. Processed data for plotting Activation Energy.

Processed data for Activation Energy plot												
	Temp. °C (°C)	Temp. K (K)	Δ Temp (%)	1/T (K ⁻¹)	Initial rate (dm ³ mol ⁻¹ s ⁻¹)	Δ Rate (%)	Δ Rate (Absolute)	Rate constant (k) (dm ³ mol ⁻¹ s ⁻¹)	Δ k (Absolute)	ln(k)	Δ ln(k)	
1	14,13	287,13	0,35	0,0034827	0,00801	2,2	0,00018	2,0E-03	4,4E-05	-6,21	0,022	
2	21,40	294,40	0,23	0,0033967	0,00295	2,2	6,5E-05	7,4E-04	1,6E-05	-7,21	0,022	
3	30,97	303,97	0,16	0,0032898	0,00570	2,2	0,00013	1,4E-03	3,1E-05	-6,55	0,022	
4	37,80	310,80	0,13	0,0032175	0,00676	2,2	0,00015	1,7E-03	3,7E-05	-6,38	0,022	
5	51,17	324,17	0,098	0,0030848	0,01090	2,2	0,00024	2,7E-03	6,0E-05	-5,90	0,022	

To convert the temperature in Celsius to Kelvin I simply added 273 to my value, and since this is a constant the uncertainty does not play a role, hence the temperature in Kelvin is written as 2 decimal places.

$$30.97 + 273 = 303.97 \text{ K (2 d. p.)}$$

$$\% \text{ uncertainty of temperature} = \frac{.05}{30.97} * 100 = .16\% \text{ (2 s. f.)}$$

$\frac{1}{T}$ in Kelvin is needed to plot the activation energy.

$$\frac{1}{T} = \frac{1}{303.97} = .0032898 \text{ K}^{-1} \text{ (5 s. f.)}$$

This is displayed as 5 significant figures since that is the least number in the calculation. The initial rate and its uncertainties are from Figure 6 and Table 3, respectively. Since the theoretical uncertainty at $t=0$ s is infinitely big (division by zero), I use the average uncertainty for the rest of my domain. This turns out to be 2.2% for all five temperatures. The percentage uncertainty of k is the same as the percentage uncertainty in the initial rate.

$$\text{Abs. uncertainty in k} = \frac{2.2}{100} * 1.4 * 10^{-3} = \pm 3.1 * 10^{-5} \text{ (2 s. f.)}$$

When taking the natural logarithm of the rate constant (k), the answer is displayed in the same number of decimal places as there are significant figures in the number you are taking the logarithm of. The uncertainty of the natural logarithm of a number is approximated as $\Delta \ln(k) = \frac{\Delta k}{k}$

$$\ln(1.4 \times 10^{-3}) \text{ (2 s.f.)} = -6.55 \text{ (2 d.p.)}$$

$$\Delta \ln(1.4 \times 10^{-3}) = \frac{3.1 \times 10^{-5}}{1.4 \times 10^{-3}} = \pm .022 \text{ (2 s.f.)}$$

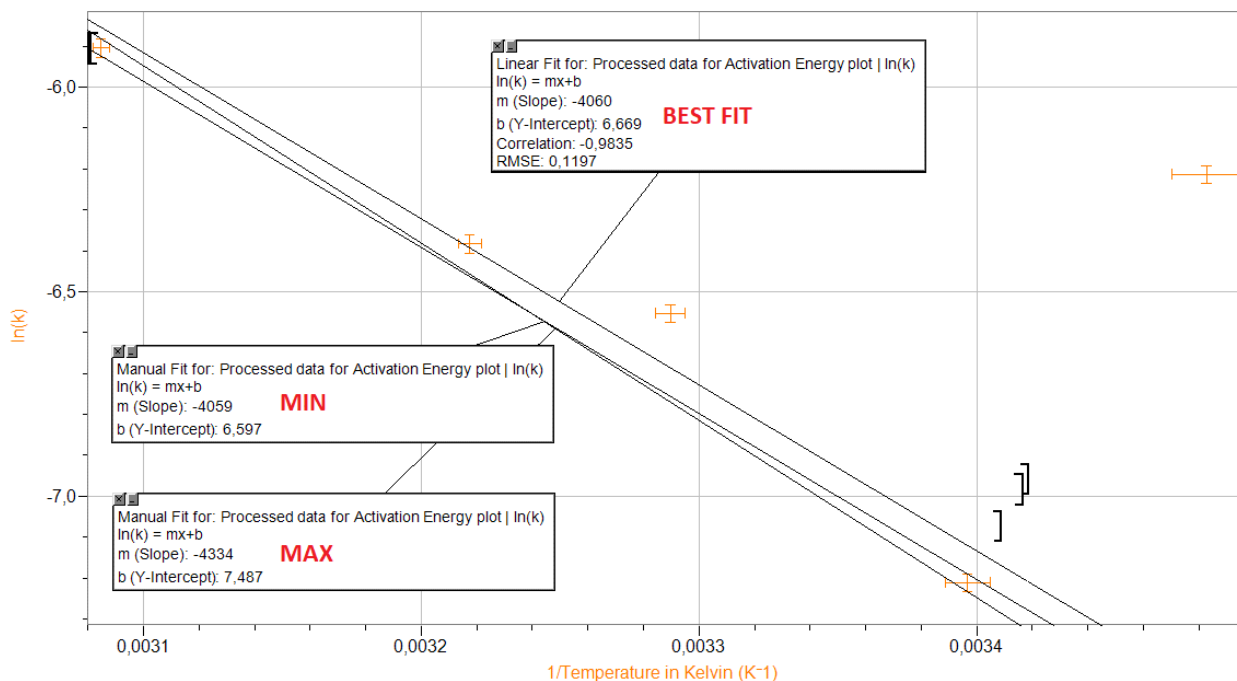


Figure 7. $\ln(k)$ vs $1/T$. Shows max, min, and best-fit lines.

Table 5. Showing gradient and activation energy,

	Gradient	E_a (J mol ⁻¹)
Max	-4334	36 016
Best fit	-4060	33 739
Min	-4059	33 730

$$\Delta E_a = \frac{\text{max} - \text{min}}{2} = \frac{(36016 - 33730)}{2} = 1142.6 \text{ J mol}^{-1} \approx 1.1 \text{ kJ mol}^{-1} \text{ (2 s.f.)}$$

$$E_a = 33.7 \pm 1.1 \text{ kJ mol}^{-1}$$

⁷ "App A: Propagation of Logarithms." Capuphysics.Ca. Last modified 2020. Accessed October 24, 2020. <http://phys114115lab.capuphysics.ca/App%20A%20-%20uncertainties/appA%20propLogs.htm>.

CONCLUSION

Based on the findings of this investigation I conclude that the initial rate increases if the temperature of the reactants increases. The relationship between the natural logarithm of the rate constant and 1 divided by the temperature in Kelvin is linear. I have also found the activation energy for the reaction between sodium carbonate and dilute hydrochloric acid to be $33.7 \pm 1.1 \text{ kJ mol}^{-1}$. Large positive activation energies such as this tell me that the initial rate will increase drastically at higher energies. After searching for Activation Energy databases online, I was unable to find a literary value for this reaction in particular. Therefore, I am unable to calculate my percentage error.

Even though I am unable to compare my value to a literary value, I can still say a lot about it from the data I collected. Even though the range between my values for the volume of carbon dioxide gas produced is quite big, the experimental uncertainty is low. Table 4 and Figure 5 show clearly that the initial rates are bigger when the temperature of the reactants is higher, confirming my research hypothesis, which refers back to the figure in the introduction regarding Maxwell – Boltzmann energy distribution and temperature. My data confirm the theory by simply looking at the trends in the data.

EVALUATION

Method, errors, and uncertainties

When calculating the activation energy, the values for the error bars in Figure 7 is not experimental uncertainty, but rather the random uncertainty from the equipment. Due to the nature of the experiment, with many different data points, it was not feasible to use experimental uncertainties. One could calculate the initial rate for all the 15 trials individually and plot all these data points to find the activation energy. The value would be the same (at least to 1 d.p. which is used in my answer), but this would make it possible to use the R and R² values to say something about the precision of the experiment. Nevertheless, one should note that the experimental uncertainty of E_a is only 3.3% $\left(\frac{1.1}{33.7} * 100\right)$. The uncertainty in the equipment is 2.2% (Table 3), so they are within reason of each other.

The method has undergone development for the better during the initial testing at the lab. This helped improve some things, such as pouring the hydrochloric acid from a beaker instead of a pipette. This allowed for the pouring to go quicker. This is important since getting the rubber bung in place quickly to not have gas escape the system. Performing tests to find suitable concentrations was also important. Nevertheless, the reaction proceeds from when the first drop of HCl is in, but the measuring is not started until the rubber bung is in position. During the time between the start of the reaction and the start of measuring, gas is lost to the surroundings. This is because my system is flawed in the sense that it is not an isolated system. The result of this is a systematically lower reading of the volume of gas produced. This has two main consequences and one minor:

- I. **The effect on ln(k):** Measuring a systematically lower volume means that the initial rate will be lower. This means that the rate constant (k) will also be lower, which leads to a more negative value for ln(k) since the rate is between 0 and 1. The result of this is that the gradient would be less steep, decreasing the calculated activation energy. One has to note that if the amount of gas lost would be equal for all trials, it would not have any effect on the activation energy since we are calculating using the gradient, so a translation in y-direction would not matter. Regardless, the amount of gas lost is not the same, since when the temperature is higher, the reaction would proceed further

before the rubber bung is in place, compared to lower temperatures, hence losing a different amount of gas each time.

- II. **The effect on $1/T$:** The reaction used in the experiment is exothermic, which means that heat is released when the reaction proceeds. In my paper, I have assumed that there is no energy lost to surroundings, but the system will converge towards the temperature of the surroundings (room temperature). If the heat loss is not accounted for, which it is not, the temperature used in the calculations might not be representative of the real temperature. This means that the values for $1/T$ are systematically too big, which then leads to a less steep gradient, decreasing the calculated activation energy further. The amount of error here is also not the same for all temperatures. If it were so, it would only be a translation of the graph in the x-direction. At higher temperatures, more energy will be lost to surroundings, so the *change* in temperature is not the same for different initial temperatures.
- III. Many of the factors in the Arrhenius equation is temperature dependent. This means that any error in temperature also leads to errors in the other values. This is beyond the scope of the curriculum and is going further into multivariable calculus and thermochemistry. The previously mentioned errors are commented on as if they are independent of each other.

Weaknesses

As mentioned earlier in the paper, I consider T_1 to be an outlier, and therefore, I did not use it in calculating the activation energy. With three trials on each temperature, it gave me 15 data points to consider. It was based on my data, that I chose to disregard T_1 completely. Nevertheless, it is likely that the three trials done on temperatures around 10°C are the ones that yielded the most *accurate* data. This is because of how slow the rate is, which means that loss of gas before the measurement has started is minimal. This demonstrates how the previously mentioned open system can lead to less accurate data when the rate is higher.

Strengths

A strength in the investigation is the large amount of data collected. The investigation includes enough data to reasonably draw conclusions about trends, as well as calculating the activation energy. The experiment itself is also not difficult to perform, and it is fully possible to collect even more data. The experiment also includes reasonably harmless chemicals (at least when using a diluted acid such as I did). The method developed works on a vast number of reactions where gas is one of the products, so one can change the chemicals and use my method to calculate the activation energy for other reactions. The method is easily repeatable and can be developed further to battle the aforementioned loss of gas.

Improvements

The main improvement of the experiment is to create an isolated system where the reaction will follow the ideal gas law as well as proceed without energy loss. There are different ways of achieving this, but this alone would greatly improve the accuracy of the results. Preventing loss of gas would allow the data to be both more precise and more accurate. If I had more time, I would no doubt perform the trials for T_1 over again and see if it then follows the linear trend. If it does not do that, it might be necessary to limit the conclusion to only apply for certain temperatures.

Another improvement would be to use a reaction with an already known activation energy to calculate the percentage error. Without this, it is very difficult to say anything about the accuracy of my findings. There is also quite the spread of initial temperatures even though the goal was $3 \times (10-20-30-40-50)$ degrees Celsius. Using more time to carefully reach the desired temperatures would yield more precise findings.

APPENDIX A – RAW DATA

Table 6. Raw data for temperatures 1, 2, and 3. T_0 is the initial temperature. All the volumes in Table 6 are the volume of carbon dioxide gas (displaced water) after X seconds.

	T1: 1	T1: 2	T1: 3	T2: 1	T2:2	T2:3	T3:1	T3:2	T3:3
T_0 in °C ($\pm .05$ °C)	12.60	14.00	15.80	21.50	21.40	21.30	31.00	31.80	30.10
3s ($\pm .05$ ml)	2.55	11.05	2.90	1.00	1.25	0.80	3.60	3.70	3.20
6s ($\pm .05$ ml)	5.05	12.15	9.00	3.00	5.50	3.25	9.10	8.50	5.40
9s ($\pm .05$ ml)	5.30	13.15	10.60	5.00	6.40	3.45	9.60	9.30	6.10
12s ($\pm .05$ ml)	5.90	14.35	11.00	6.00	6.90	3.70	10.20	10.00	7.10
15s ($\pm .05$ ml)	6.25	14.95	11.75	6.50	7.50	4.10	10.90	10.50	7.85
18s ($\pm .05$ ml)	6.85	15.65	12.30	7.30	8.30	4.45	11.40	11.45	8.30
21s ($\pm .05$ ml)	7.10	16.15	13.00	8.00	9.00	4.90	12.00	12.15	8.70
24s ($\pm .05$ ml)	7.60	16.75	13.70	8.30	9.60	5.05	12.35	12.85	9.70
27s ($\pm .05$ ml)	8.35	17.35	14.50	8.70	10.10	5.50	13.00	13.30	10.40
30s ($\pm .05$ ml)	8.30	18.15	14.60	9.40	10.80	5.90	13.45	14.10	11.00

Table 7. Raw data for temperatures 4 and 5. T_0 is the initial temperature All the volumes in Table 7 are the volume of carbon dioxide gas (displaced water) after X seconds.

	T4:1	T4:2	T4:3	T5:1	T5:2	T5:3
T_0 in °C ($\pm .05$ °C)	38.20	37.90	37.30	51.00	52.00	50.50
3s ($\pm .05$ ml)	2.50	3.35	4.20	2.00	4.00	4.00
6s ($\pm .05$ ml)	7.00	6.15	4.40	9.05	13.70	12.60
9s ($\pm .05$ ml)	7.40	6.65	4.60	10.30	14.10	12.80
12s ($\pm .05$ ml)	7.50	7.05	4.95	11.00	14.10	13.20
15s ($\pm .05$ ml)	7.55	7.05	4.95	11.75	14.25	13.20
18s ($\pm .05$ ml)	7.60	7.30	5.10	12.20	14.70	13.40
21s ($\pm .05$ ml)	7.75	7.55	5.35	12.65	14.90	13.75
24s ($\pm .05$ ml)	7.75	7.70	5.55	13.20	15.00	13.75
27s ($\pm .05$ ml)	7.80	8.05	5.60	13.50	15.10	14.00
30s ($\pm .05$ ml)	7.85	8.05	5.60	14.50	15.20	14.20

APPENDIX B – PROCESSED DATA

Temperature 1													
	Time (s)	V(CO ₂) (ml)	n(CO ₂) (mol)	[Na ₂ CO ₃] (mol dm ⁻³)	1/[Na ₂ CO ₃] (mol dm ⁻³) ⁻¹	ΔV (%)	Temp. (°C)	ΔT (%)	Δn(CO ₂) (Absolute)	Na ₂ CO ₃ remaining (mol)	ΔNa ₂ CO ₃ (%)	Δ[Na ₂ CO ₃] (Absolute)	Δ[Na ₂ CO ₃] (%)
1	0,0	0,00	0,00000	1,0	1,000		14,13	0,35		1,00E-02			
2	3,0	5,50	0,00023	0,98	1,024	0,91	14,13	0,35	2,9E-06	9,77E-03	2,0	0,021	2,2
3	6,0	8,73	0,00037	0,96	1,038	0,57	14,13	0,35	3,4E-06	9,63E-03	2,0	0,021	2,2
4	9,0	9,68	0,00041	0,96	1,042	0,52	14,13	0,35	3,5E-06	9,59E-03	2,0	0,021	2,2
5	12,0	10,42	0,00044	0,96	1,046	0,48	14,13	0,35	3,6E-06	9,56E-03	2,0	0,021	2,2
6	15,0	10,98	0,00046	0,95	1,048	0,46	14,13	0,35	3,7E-06	9,54E-03	2,0	0,021	2,2
7	18,0	11,60	0,00049	0,95	1,051	0,43	14,13	0,35	3,8E-06	9,51E-03	2,0	0,021	2,2
8	21,0	12,08	0,00051	0,95	1,053	0,41	14,13	0,35	3,9E-06	9,49E-03	2,0	0,021	2,2
9	24,0	12,68	0,00053	0,95	1,056	0,39	14,13	0,35	4,0E-06	9,47E-03	2,0	0,021	2,2
10	27,0	13,40	0,00056	0,94	1,060	0,37	14,13	0,35	4,1E-06	9,44E-03	2,1	0,021	2,3
11	30,0	13,68	0,00057	0,94	1,061	0,37	14,13	0,35	4,1E-06	9,43E-03	2,1	0,021	2,3

Temperature 2													
	Time (s)	V(CO ₂) (ml)	n(CO ₂) (mol)	[Na ₂ CO ₃] (mol dm ⁻³)	1/[Na ₂ CO ₃] (mol dm ⁻³) ⁻¹	ΔV (%)	Temp. (°C)	ΔT (%)	Δn(CO ₂) (Absolute)	Na ₂ CO ₃ remaining (mol)	ΔNa ₂ CO ₃ (%)	Δ[Na ₂ CO ₃] (Absolute)	Δ[Na ₂ CO ₃] (%)
1	0,0	0,00	0,00000	1,0	1,000		21,4	0,23		1,00E-02			
2	3,0	1,02	0,00004	1,0	1,004	4,9	21,4	0,23	2,1E-06	9,96E-03	1,9	0,021	2,1
3	6,0	3,92	0,00016	0,98	1,016	1,3	21,4	0,23	2,4E-06	9,84E-03	2,0	0,021	2,2
4	9,0	4,95	0,00020	0,98	1,021	1,0	21,4	0,23	2,5E-06	9,80E-03	2,0	0,021	2,2
5	12,0	5,53	0,00023	0,98	1,023	0,90	21,4	0,23	2,6E-06	9,77E-03	2,0	0,021	2,2
6	15,0	6,03	0,00025	0,98	1,025	0,83	21,4	0,23	2,6E-06	9,75E-03	2,0	0,021	2,2
7	18,0	6,68	0,00027	0,97	1,028	0,75	21,4	0,23	2,7E-06	9,73E-03	2,0	0,021	2,2
8	21,0	7,30	0,00030	0,97	1,031	0,68	21,4	0,23	2,7E-06	9,70E-03	2,0	0,021	2,2
9	24,0	7,65	0,00031	0,97	1,032	0,65	21,4	0,23	2,8E-06	9,69E-03	2,0	0,021	2,2
10	27,0	8,10	0,00033	0,97	1,034	0,62	21,4	0,23	2,8E-06	9,67E-03	2,0	0,021	2,2
11	30,0	8,70	0,00036	0,96	1,037	0,57	21,4	0,23	2,9E-06	9,64E-03	2,0	0,021	2,2

Temperature 3													
	Time (s)	Temp. (°C)	ΔT (%)	V(CO ₂) (ml)	ΔV (%)	n(CO ₂) (mol)	Δn(CO ₂) (Absolute)	Na ₂ CO ₃ remaining (mol)	ΔNa ₂ CO ₃ (%)	[Na ₂ CO ₃] (mol dm ⁻³)	Δ[Na ₂ CO ₃] (%)	Δ[Na ₂ CO ₃] (Absolute)	
1	0,0	30,97	0,16	0,00		0,00000		1,00E-02			1,0		
2	3,0	30,97	0,16	3,50	1,4	0,00014	2,2E-06	9,86E-03	1,9	0,99	2,1	0,021	
3	6,0	30,97	0,16	7,70	0,65	0,00030	2,5E-06	9,70E-03	2,0	0,97	2,2	0,021	
4	9,0	30,97	0,16	8,30	0,60	0,00033	2,5E-06	9,67E-03	2,0	0,97	2,2	0,021	
5	12,0	30,97	0,16	9,10	0,55	0,00036	2,6E-06	9,64E-03	2,0	0,96	2,2	0,021	
6	15,0	30,97	0,16	9,80	0,51	0,00039	2,6E-06	9,61E-03	2,0	0,96	2,2	0,021	
7	18,0	30,97	0,16	10,40	0,48	0,00041	2,6E-06	9,59E-03	2,0	0,96	2,2	0,021	
8	21,0	30,97	0,16	11,00	0,45	0,00044	2,7E-06	9,56E-03	2,0	0,96	2,2	0,021	
9	24,0	30,97	0,16	11,60	0,43	0,00046	2,7E-06	9,54E-03	2,0	0,95	2,2	0,021	
10	27,0	30,97	0,16	12,20	0,41	0,00048	2,8E-06	9,52E-03	2,0	0,95	2,2	0,021	
11	30,0	30,97	0,16	12,90	0,39	0,00051	2,8E-06	9,49E-03	2,0	0,95	2,2	0,021	

Temperature 4													
	Time (s)	V(CO ₂) (ml)	n(CO ₂) (mol)	[Na ₂ CO ₃] (mol dm ⁻³)	1/[Na ₂ CO ₃] (mol dm ⁻³) ⁻¹	ΔV (%)	Temp. (°C)	ΔT (%)	Δn(CO ₂) (Absolute)	Na ₂ CO ₃ remaining (mol)	ΔNa ₂ CO ₃ (%)	Δ[Na ₂ CO ₃] (Absolute)	Δ[Na ₂ CO ₃] (%)
1	0,0	0,00	0,00000	1,0	1,000		37,8	0,13		1,00E-02			
2	3,0	3,35	0,00013	0,99	1,013	1,5	37,8	0,13	2,1E-06	9,87E-03	1,9	0,021	2,1
3	6,0	5,85	0,00023	0,98	1,023	0,85	37,8	0,13	2,2E-06	9,77E-03	2,0	0,021	2,2
4	9,0	6,22	0,00024	0,98	1,025	0,80	37,8	0,13	2,3E-06	9,76E-03	2,0	0,021	2,2
5	12,0	6,50	0,00025	0,97	1,026	0,77	37,8	0,13	2,3E-06	9,75E-03	2,0	0,021	2,2
6	15,0	6,52	0,00025	0,97	1,026	0,77	37,8	0,13	2,3E-06	9,75E-03	2,0	0,021	2,2
7	18,0	6,67	0,00026	0,97	1,027	0,75	37,8	0,13	2,3E-06	9,74E-03	2,0	0,021	2,2
8	21,0	6,88	0,00027	0,97	1,027	0,73	37,8	0,13	2,3E-06	9,73E-03	2,0	0,021	2,2
9	24,0	7,00	0,00027	0,97	1,028	0,71	37,8	0,13	2,3E-06	9,73E-03	2,0	0,021	2,2
10	27,0	7,15	0,00028	0,97	1,028	0,70	37,8	0,13	2,3E-06	9,72E-03	2,0	0,021	2,2
11	30,0	7,17	0,00028	0,97	1,029	0,70	37,8	0,13	2,3E-06	9,72E-03	2,0	0,021	2,2

Temperature 5													
	Time (s)	V(CO ₂) (ml)	n(CO ₂) (mol)	[Na ₂ CO ₃] (mol dm ⁻³)	1/[Na ₂ CO ₃] (mol dm ⁻³) ⁻¹	ΔV (%)	Temp. (°C)	ΔT (%)	Δn(CO ₂) (Absolute)	CO ₂ remain (mol)	ΔNa ₂ CO ₃ (%)	Δ[Na ₂ CO ₃] (Absolute)	Δ[Na ₂ CO ₃] (%)
1	0,0	0,00	0,00000	1,0	1,000		51,17	0,098		1,00E-02			
2	3,0	3,33	0,00012	0,99	1,013	1,5	51,17	0,098	2,0E-06	9,88E-03	1,9	0,021	2,1
3	6,0	11,78	0,00044	0,96	1,046	0,42	51,17	0,098	2,3E-06	9,56E-03	2,0	0,021	2,2
4	9,0	12,40	0,00046	0,95	1,048	0,40	51,17	0,098	2,3E-06	9,54E-03	2,0	0,021	2,2
5	12,0	12,77	0,00047	0,95	1,050	0,39	51,17	0,098	2,3E-06	9,53E-03	2,0	0,021	2,2
6	15,0	13,07	0,00049	0,95	1,051	0,38	51,17	0,098	2,3E-06	9,51E-03	2,0	0,021	2,2
7	18,0	13,43	0,00050	0,95	1,052	0,37	51,17	0,098	2,3E-06	9,50E-03	2,0	0,021	2,2
8	21,0	13,77	0,00051	0,95	1,054	0,36	51,17	0,098	2,4E-06	9,49E-03	2,0	0,021	2,2
9	24,0	13,98	0,00052	0,95	1,055	0,36	51,17	0,098	2,4E-06	9,48E-03	2,0	0,021	2,2
10	27,0	14,20	0,00053	0,95	1,056	0,35	51,17	0,098	2,4E-06	9,47E-03	2,0	0,021	2,2
11	30,0	14,63	0,00054	0,95	1,057	0,34	51,17	0,098	2,4E-06	9,46E-03	2,0	0,021	2,2