Investigating the Effect of Temperature on the Rate Constant of the Decomposition of Aqueous Hydrogen Peroxide.

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IB Chemistry HL
Internal Assessment

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Contents

1 Introduction

The reaction of hydrogen peroxide, H_2O_2, decomposes to form oxygen gas and water. Although this reaction is thermodynamically favourable to the products side, it will proceed at an extremely-slow rate at room temperature, unless catalyzed:

$$2\,H_2O_{2(aq)} \longrightarrow 2\,H_2O_{(l)} + O_{2(g)}$$
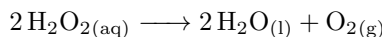
In this investigation, potassium iodide (KI) was used as a catalyst so that the reaction (specifically, the formation of oxygen gas) inside the system canb occur at a measurable rate within a practical time frame. This investigation aims to explore how temperature impacts the rate constant for the catalyzed decomposition reaction of aqeuous hydrogen peroxide. The rate of the reaction is observed indirectly by measuring the initial rate of increase in gas pressure inside a sealed flask, as oxygen gas ($O_{2(g)}$) builds up.

1.1 Background Concepts

The collision theory states that for a chemical reaction can only occur when particles collide with energy and the correct orientation. As the temperature of the reaction system increase, reacting particles have greater average kinetic energy. This increase in the particle's collision ferquency and the increase in the probability of collisions with energy *equal or greater than* the activation energy (E_A). Thus, increasing the temperature of the reaction is expected to increase the rate of the reaction and the reaction constant. The temperature dependence of a rate constant can be modelled by the Arrhenius equation:

$$k = A \cdot e^{-\frac{E_A}{RT}} \tag{1}$$

Where k is the rate constant, A is the frequency factor, E_A is the activation energy, R is the gas constant $(8.31 \text{ J K}^{-1} \text{ mol}^{-1})$[1], and T is the temperature, in Kelvins.

Taking the natural logarithm on both sides of the equation will yield a linear graph:

$$ln(K) = -\frac{E_A}{RT} + ln(A) \tag{2}$$

Where the slope of the linear graph is $-\frac{E_A}{R}$, and the y-intercept is $ln(A)$.

As oxygen gas ($O_{2(g)}$) forms in the sealed flask of approximate constant gas volume, the pressure increases. Assuming ideal gas behaviour, the pressure should increase as n (the number of moles of gas) increases, but V (volume) stays constant:

$$PV = nRT \tag{3}$$

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[1]Value obtained from IB Chemistry Data Booklet, version 1.0 (first assessment 2025).

$$\therefore P \propto n \tag{4}$$

Given that the initial concentration of H_2O_2 and the amount of catalyst added were held constant across all trials, the calculated rate constant can be compared across temperature levels.

$$* * *$$

As a result, the research question for this investigation is:

How does the temperature affect the rate constant for the decomposition of aqueous hydrogen peroxide, determined from the initial rate of increase of gas pressure in a sealed flask?

1.2 Hypothesis

Given that the Arrhenius rate constant is dependent on the temperature, I hypothesize that increasing the temperature will cause the rate constant for the decomposition of aqueous hydrogen peroxide, H_2O_2, to increase exponentially.

2 Research Design

2.1 Variables

Independent variable: Temperature of the reaction system. The H_2O_2 in the sealed flask was equilibrated to the target temperature using a water bath and heat plate before the start of each trial. The temperature was monitored using a Vernier Temperature Probe before and during the trials. The trials were only started once the water bath temperature reached within 1 °C of the target temperature.

Dependent variable: Rate of the decomposition reaction of H_2O_2 and KI.

Controlled variable: Initial concentration of H_2O_2 (mol dm^{-3}), total volume of gas space in the sealed flask, environmental conditions (temperature, humidity), time interval between pressure readings, the same apparatus setup (same Vernier pressure sensor used for all measurements), and data-collection settings.

2.2 Materials

- (1x) Bottle of 3% hydrogen peroxide, H_2O_2 (aqueous)

- (1x) Bottle of potassium iodide, KI (solid)

- (1x) Jug of distilled water

- (1x) 1000 mL beaker (waste beaker)

- (2x) 600 mL beakers

  1. (1x) for ice bath

  2. (1x) for H_2O_2 solution

- (1x) 250 mL flask (for experiment, to be placed in water bath)

- (1x) 250 mL beaker (for H_2O_2 solution)

- (1x) 100 mL beaker (for KI solution)

- (1x) Glass bowl (for water bath)

- (1x) Rubber stoppers (with holes and pipes)

- (1x) Vernier Gas Pressure Sensor

- (1x) Vernier Stainless Steel Temperature Probe

- (1x) Vernier LabQuest

- (1x) 25 mL Pipette + suction bulb

- (1x) 10 mL graduated cylinder (for measuring distilled water)

- (1x) Digital balance

- (1x) Metal stick from ring stand

- (1x) Safety goggles

- (1x) Lab coat

2.3   Experimental Design

This experiment was designed to isolate the temperature of the water bath as the sole independent variable affecting the rate constant for the KI-catalyzed decomposition reaction of aqueous hydrogen peroxide. Oxygen gas produced during the reaction increased the pressure inside a sealed 250 mL flask. Thus, the increase in the rate of the initial pressure value was used to determine the rate constant at each temperature. A water bath (wide glass bowl on heat plate) was used to equilibrate the reaction system to within 1°C of the target temperature, with ice available in a beaker nearby to lower temperatures when required. The mass of KI were pre-measured and recorded before data collection, and sealed with plastic wrap and rubber band.

2.4 Procedure

2.4.1 Part I: Setup

1. Obtain safety goggles and lab coat.

2. Gather the required items from *section 2.2* to work station.

3. Assemble the pressure measurement setup:

   - Connect the Vernier Gas Pressure sensor to the LabQuest

   - Connect the airtight plastic tube to the pressure sensor.

   - Connect the plastic tubing to the rubber stopper.

   - Close the valve on the rubber stopper.

4. Secure the 250 mL flask on the ring stand using a ring clamp, so that it remains stable during the data collection.

5. Add 25 mL of distilled water to the 250 mL flask for setup purposes.

6. To prepare the water bath, place the glass bowl on the hot plate and add water to a level so that it just submerges the 25 mL water inside the flask. This will represent the hydrogen peroxide during the experiment.

7. Draw a horizontal line on the neck of the reaction flask using a marker to standardize the insertion depth of the rubber stopper in every trial.

   - **<u>Note:</u>** Before inserting the rubber stopper each time, add a few drops of water on fingers, and rub the sides of the rubber stopper to improve the sealing.

8. Ensure the temperature probe is not touching the bottom of the glass bowl or the sides of the flask. Secure the temperature probe using a ring clamp (to standardize the placement between trials)

9. Set the LabQuest to record at *5 samples / second*, for a total of *60 seconds* for each trial.

2.4.2 Part II: Preparation of materials

1. Pour a large amount of aqueous H_2O_2 into a clean 600 mL beaker to use as the master solution for all trials. Excess can be poured back using a funnel.

2. Prepare potassium iodide portions for each trial:

   (a) Using a digital scale, weigh 0.30 g of solid KI into individual plastic cups.

   (b) Label each cup with its corresponding temperature level and trial number.

(c) Seal each cup using a piece of plastic film, and secure it with rubber band to reduce exposure to moisture from air.

3. Using another clean 600 mL beaker, fill with ice. This will be used to lower the temperature of the water bath for lower temperature levels.

2.4.3   Part III: Calibration

1. With the apparatus assembled, open the valve on the rubber stopper so that the pressure sensor is open to the atmosphere. Record the atmospheric pressure for 10 seconds and record the average pressure in kPa.

2. Rinse the 25 mL pipette with aqueous H_2O_2 to avoid contaminatino, then dispose into the waste beaker.

Note: An airtight-sealing calibration was not conducted because the experiment relies on finding the change in pressure over time. In the case of a minor leak, the pressure readings would be consistently lower than the actual pressure, which does not affect the rate of change in pressure and the rate constant.
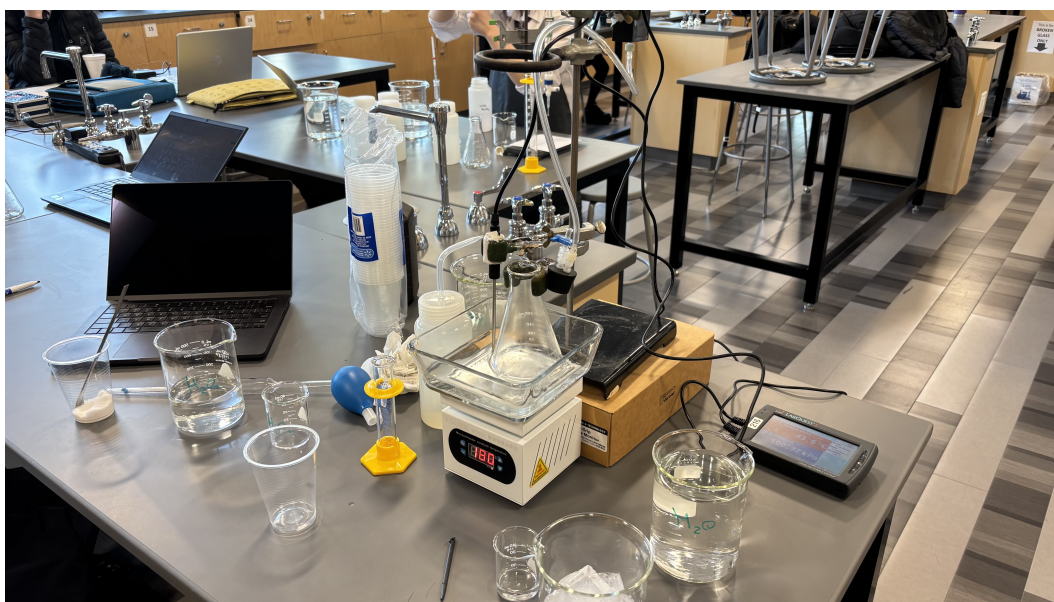
Figure 1: Apparatus setup.

2.4.4   Part IV: Experiment

1. Adjust the water bath temperature to the target temperature, either by using the hot plate or by adding ice (depending on temperature level).

2. Pipette 25 mL of H_2O_2 to a clean 250 mL beaker. Once the temperature of the water bath reaches within 1 °C of the target temperature, pour the H_2O_2 into the reaction flask. Keep the reaction flask in the water bath to maintain consistency.

3. Measure 5 mL of distilled water using a 10 mL graduated cylinder, and pour into the plastic cup containing the pre-weighed KI for the trial. Stir to dissolve the KI. Repeat twice, so that there is a total of 10 mL of KI solution.

4. Start the data collection and collect a 3 second baseline with the flask sealed. Then, remove the rubber stopper, and quickly add the KI solution into the reactino flask, and immediately seal the flask with the rubber stopper (with water on sides of flask to improve seal).

5. Swirl the flask gently for *5 seconds*, then keep the flask still for the remainder of the run.

6. After data collection ends, save the run, and record the LabQuest run number in the data table with the corresponding trial.

7. Dispose the solution into the waste beaker, and rinse the reaction flask once using tap water, then rinse again with distilled water.

8. Repeat *steps 1-7* for each trial at each temperature level, for a total of *40 trials*.

2.4.5 Part V: Cleanup

1. Disconnect the gas pressure sensor and temperature probe from the LabQuest.

2. Save the file on the LabQuest, and download the data to a computer.

3. Neutralize the waste solution by adding a small amount of sodium thiosulfate, then dispose the waste solution down the drain with running water.

4. Return used glassware to the dirty bin, and return all equipment.

Note: If table turns yellow, wipe down with a paper towel, some water, and a few crystals of sodium thiosulfate.

3 Data Collection

3.1 Data Tables

3.2 Sources of Uncertainty

To reduce random errors, 5 trials were conducted at each temperature level and averaged. Other variables, such as initial H_2O_2 concentration and volume, mass of KI, apparatus setup, and sealing method were all kept constant across all runs so that differences in the initial pressure-increase rate can be attributed primary to temperature.

4   Data Processing

4.1   Uncertainty Propagation

The uncertainty values for temperature and pressure were obtained from specifications of the equipment used, and the smallest scale on the digital balance was used as the uncertainty of mass: ± 0.01 g. A 25 mL volunmetric pipette was used to obtain the H_2O_2 for all trials, but the exact volumes delivered were not confirmed with a graduated cylinder. Thus, the pipette's tolerance was used as the volume uncertainty: ± 0.06 mL. Time was recorded automatically by the LabQuest, so its uncertainty was assumed negligible relative to pressure variation throughout the experiment.

Tool	Uncertainty
Vernier Stainless Steel Temperature Probe	± 0.1 °C at 0 °C, ± 0.5 °C at 100 °C
Vernier Gas Pressure Sensor	± 4 kPa
Digital Balance	± 0.01 g
Volunmetric Pipette	± 0.06 mL

Table 1: Summary of uncertainties by tool.

Given that the Vernier documentation provides two uncertainty values for the temperature probe, linear interpolation was used for the uncertainty of the device:

$$\Delta T(x) = 0.20 + \frac{0.50 - 0.20}{100} \cdot x \tag{5}$$

Where x is the measured temperature obtained from the temperature probe (in Celsius), and ΔT is the uncertainty in Kelvin [2].

4.1.1   Uncertainty in rate constant

The rate constant was calculated as the slope of a linear best-fit trendline to the pressure-time graph over a fixed *15 second* interval, starting at the first continuous rise in pressure after the rubber stopper was replaced [3]. The reaction rate equation for the decomposition reaction of hydrogen peroxide (H_2O_2) and potassium iodide (KI) can be expressed in the general form, where r is the reaction rate and k is the rate constant:

$$r = k[H_2O_2]^m[I^-]^n \tag{6}$$

Given that the moles of H_2O_2 and the amount of KI were held constant for all trials, the reaction rate is directly proportional to the rate constant k with temperature. Moreover, according to the ideal gas relationship ($PV = nRT$), pressure inside the sealed flask is proportional to the moles of O_2 produced:

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[2]Uncertainty is not affected by the conversion between Celsius and Kelvin.

[3]**First continuous rise:** The first datapoint was counted as the start interval after a consecutive rise in the next adjacent 3 datapoints

$$P \propto n \tag{7}$$

Thus, an apparent rate constant k_{app} can be defined using the initial rate of pressure increase:

$$k_{app} = \frac{\Delta P}{\Delta t} \tag{8}$$

$$k_{app} \propto k \tag{9}$$

As there are 5 trials per temperature level, a mean apparent rate constant was calculated to represent the rate constant at each temperature::

$$\bar{k}_{\mathrm{app}} = (\frac{1}{n}) \cdot \sum_{i=1}^{n} k_{\mathrm{app},i}, \quad (n = 5) \tag{10}$$

The random uncertainty in the mean k_{app} value was then calculated:

$$\Delta \bar{k}_{\mathrm{app}} = \frac{\sigma}{\sqrt{n}} \tag{11}$$

Where σ is the standard deviation of the 5 k_{app} values, and n is the number of trials (5). This was included because random uncertainties (caused by small variations in, for example, plastic film sealing, mixing time, etc.) can be reduced by taking average, but systematic uncertainties (i.e. constant volunmetric tolerance from using the same pipette for all trials) does not average out.

4.2 Processed Data

Temp (°C)	Trial	Average temp (°C)	Average temp (K)	Mass of KI (g)	Start window (s)	End window (s)	Initial rate (kPa/s)	Avg. initial rate (kPa/s)	Initial rate SD (kPa/s)
15	1	14.75	287.90	0.30	26.6	41.6	0.00594	0.01023 ± 0.00194	0.00434
	2	15.70	288.85	0.29	40.4	55.4	0.00817		
	3	14.35	287.50	0.32	30.0	45.0	0.01237		
	4	15.10	288.25	0.32	30.0	45.0	0.01676		
	5	14.86	288.01	0.31	20.2	35.2	0.00792		
20	1	19.00	292.15	0.30	31.8	46.8	0.01397	0.01406 ± 0.00223	0.00498
	2	20.95	294.10	0.28	17.2	32.2	0.00864		
	3	21.15	294.30	0.29	25.8	40.8	0.01510		
	4	19.55	292.70	0.31	30.0	45.0	0.02171		
	5	19.55	292.70	0.31	24.0	39.0	0.01089		
25	1	25.50	298.65	0.29	19.0	34.0	0.01867	0.01782 ± 0.00315	0.00705
	2	25.55	298.70	0.29	20.0	35.0	0.02864		
	3	26.20	299.35	0.29	27.2	42.2	0.01631		
	4	24.65	297.80	0.28	24.0	39.0	0.01644		
	5	25.65	298.80	0.30	20.0	35.0	0.00904		
30	1	30.10	303.25	0.33	5.6	20.6	0.03811	0.03884 ± 0.00870	0.01944
	2	28.80	301.95	0.30	10.2	25.2	0.02327		
	3	31.20	304.35	0.30	11.0	26.0	0.06776		
	4	30.20	303.35	0.30	17.2	32.2	0.04581		
	5	30.90	304.05	0.29	11.4	26.4	0.01924		
35	1	35.50	308.65	0.31	8.0	23.0	0.06992	0.05442 ± 0.00600	0.01342
	2	35.55	308.70	0.31	16.8	31.8	0.05917		
	3	34.20	307.35	0.32	13.2	28.2	0.06227		
	4	35.00	308.15	0.31	6.2	21.2	0.04098		
	5	35.90	309.05	0.29	21.4	36.4	0.03975		
40	1	40.35	313.50	0.28	11.6	26.6	0.06090	0.04214 ± 0.00826	0.01847
	2	41.20	314.35	0.28	11.0	26.0	0.02914		
	3	38.90	312.05	0.29	9.6	24.6	0.02469		
	4	40.50	313.65	0.28	8.8	23.8	0.06334		
	5	38.95	312.10	0.29	10.0	25.0	0.03264		
45	1	45.25	318.40	0.29	6.6	21.6	0.04139	0.09427 ± 0.03053	0.06826
	2	43.85	317.00	0.30	16.2	31.2	0.06972		
	3	44.80	317.95	0.29	4.8	19.8	0.19417		
	4	44.60	317.75	0.29	8.0	23.0	0.13306		
	5	44.65	317.80	0.29	12.4	27.4	0.03301		
50	1	49.30	322.45	0.31	4.6	19.6	0.17295	0.10081 ± 0.02089	0.04672
	2	49.40	322.55	0.28	9.8	24.8	0.05932		
	3	48.55	321.70	0.29	11.4	26.4	0.07183		
	4	49.45	322.60	0.29	5.2	20.2	0.12192		
	5	49.80	322.95	0.29	11.2	26.2	0.07802		

Table 2: Processed data.

Note: The initial rate of pressure increase was calculated by finding the slope of the trendline of the pressure-time graph, using a fixed window of **_15 seconds_** starting from the moment the pressure sensor settles and reaction begins.

4.3 Raw Data

Note: The original raw data file obtained from the LabQuest is 300 rows by 80 columns. Due to the size of this, the raw data file can be found in the appendix, *section A.1*.

Level	Trial	Target (°C)	Target (K)	Run # (LabQuest)	Start temp (°C)	End temp (°C)	Average temp (°C)	Volume of H_2O_2 (mL)	Mass of KI (g)
1	1	15	288.15	4	14.4	15.1	14.75	25	0.30
	2			5	15.4	16	15.70		0.29
	3			6	14.7	14	14.35		0.32
	4			7	14.9	15.3	15.10		0.32
	5			8	15.32	14.4	14.86		0.31
2	1	20	293.15	48	19.3	18.7	19.00	25	0.30
	2			9	21.4	20.5	20.95		0.28
	3			10	21	21.3	21.15		0.29
	4			11	19.7	19.4	19.55		0.31
	5			12	19.3	19.8	19.55		0.31
3	1	25	298.15	13	25.2	25.8	25.50	25	0.29
	2			14	25.3	25.8	25.55		0.29
	3			15	25.7	26.7	26.20		0.29
	4			16	24.7	24.6	24.65		0.28
	5			17	25.4	25.9	25.65		0.30
4	1	30	303.15	18	29.6	30.6	30.10	25	0.33
	2			19	29.1	28.5	28.80		0.30
	3			20	30.9	31.5	31.20		0.30
	4			21	30	30.4	30.20		0.30
	5			22	30.8	31	30.90		0.29
5	1	35	308.15	23	35.6	35.4	35.50	25	0.31
	2			24	35.3	35.8	35.55		0.31
	3			25	35.1	33.3	34.20		0.32
	4			26	34.7	35.3	35.00		0.31
	5			27	35.5	36.3	35.90		0.29
6	1	40	313.15	43	39.8	40.9	40.35	25	0.28
	2			44	41.3	41.1	41.20		0.28
	3			45	40.5	37.3	38.90		0.29
	4			46	40	41	40.50		0.28
	5			47	39.1	38.8	38.95		0.29
7	1	45	318.15	33	45.6	44.9	45.25	25	0.29
	2			34	44.5	43.2	43.85		0.30
	3			35	44.8	44.8	44.80		0.29
	4			36	44.5	44.7	44.60		0.29
	5			37	45.1	44.2	44.65		0.29
8	1	50	323.15	38	49.1	49.5	49.30	25	0.31
	2			39	49.8	49	49.40		0.28
	3			40	49	48.1	48.55		0.29
	4			41	49.2	49.7	49.45		0.29
	5			42	49.7	49.9	49.80		0.29

Table 3: Temperature runs (raw data).

4.4 Example Calculation

Consider the first trial of the first temperature level, 15°C as an example (marked as red, in *table 2*). For this trial, the average temperature (taken from the start + end temperature) was 14.75°C:

$$T = 14.75°C + 274.15 = 287.9K \tag{12}$$

Given that the analysis window for the pressure-time graph is 15 seconds starting at the first continuous rise after the rubber stopper was replaced, using the data helper I programmed [4], the selected interval was:

$$t_{\text{start}} = 26.6 \text{ s}, \quad t_{\text{end}} = 41.6 \text{ s} \tag{13}$$
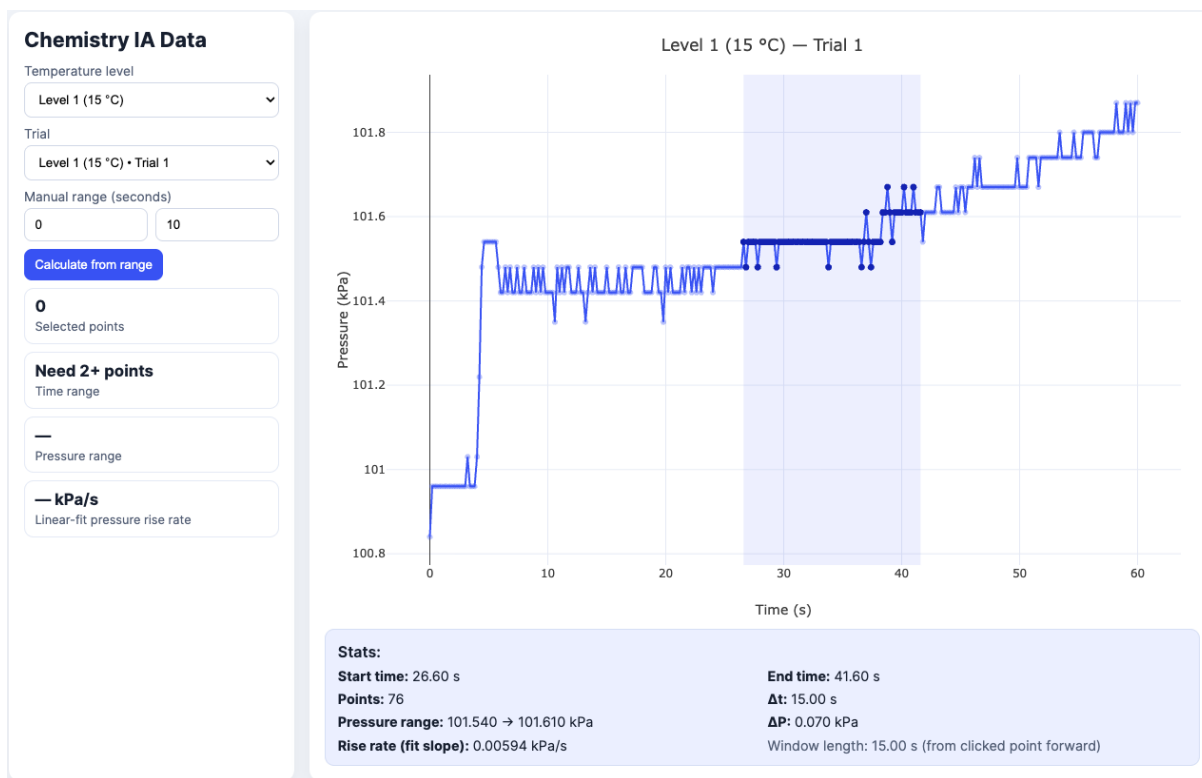

Figure 2: Data helper.

A linear regression was then fitted to the 76 datapoints in the selected window, using the linear trendline formula $P = mt + b$ in Excel, where the slope m is the apparent rate constant k_{app}:

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[4]To speed up data processing for all 40 trials, I programmed a helper that loaded all data and autoamtically generated graphs and stats using *Python* and the *Plotly.js* library.
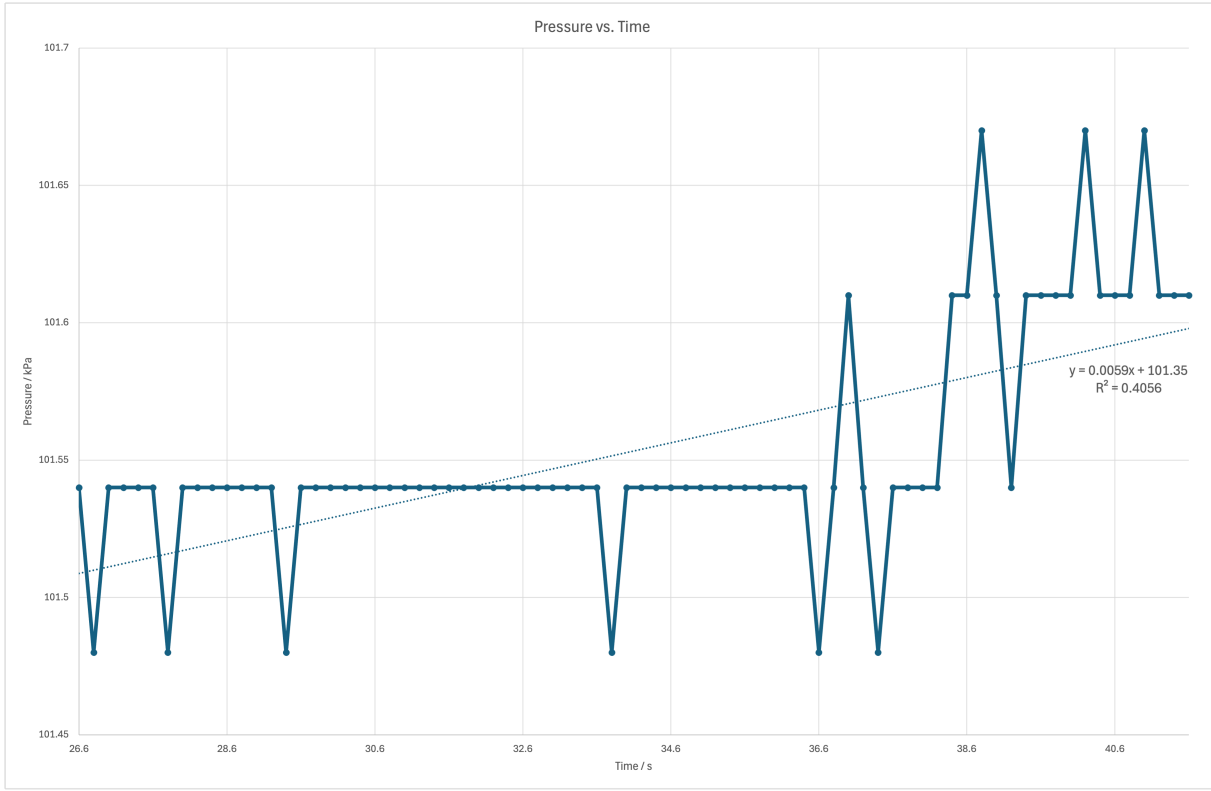
Figure 3: 15-second snapshot.

As shown in the graph above, the slope value over the time interval 26.6 s to 41.6 s was 0.0059 kPa s^{-1}. This matches the value reported for 15 °C, *trial 1* in *table 2*. The average apparent rate constant can then be calculated:

$$\overline{k_{app}} = \frac{0.00594 \text{ kPa s}^{-1} + 0.00817 \text{ kPa s}^{-1} + 0.01237 \text{ kPa s}^{-1} + 0.01676 \text{ kPa s}^{-1} + 0.00792 \text{ kPa s}^{-1}}{5} \tag{14}$$

$$\overline{k_{app}} = \frac{0.05116 \text{ kPa s}^{-1}}{5} = 0.010232 \text{ kPa s}^{-1} \tag{15}$$

The standard deviation of the five trials is 0.00434:

$$\sigma = \sqrt{\frac{1}{5}(-0.004292)^2 + (-0.002062)^2 + (0.002138)^2 + (0.006528)^2 + (-0.002312)^2} \tag{16}$$

$$\sigma = 0.004234 \text{ kPa s}^{-1} \tag{17}$$

The random uncertainty in the mean can then be calculated:

$$\Delta \overline{k_{app}} = \frac{0.00434 \text{ kPa s}^{-1}}{\sqrt{5}} = 0.00194 \text{ kPa s}^{-1} \tag{18}$$

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Thus, the rate constant for the first trial of 15 °C is:

$$k_{app} = 0.01023 \pm 0.00194 \text{ kPa s}^{-1} \tag{19}$$

* * *

The approach from above was used to calculate the apparent rate constant for the other 8 temperature levels:

Temperature level (°C)	Apparent rate constant, k_{app} (kPa s^{-1})
15	0.01023 ± 0.00194
20	0.01406 ± 0.00223
25	0.01782 ± 0.00315
30	0.03884 ± 0.00870
35	0.05442 ± 0.00600
40	0.04214 ± 0.00826
45	0.09427 ± 0.03053
50	0.10081 ± 0.02089

Table 4: Apparent rate constant.

5 Data Analysis

6 Conclusion

7 Evaluation

7.1 Strengths

7.2 Weaknesses & Limitations

References

A   Appendix

A.1   Complete Raw Data

A.2   Source Code

All source code and raw data are open-source, available to view on GitHub.