

CHE213

INNOVATION

PROJECT

Group 12

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INTRODUCTION

Investigating the Diffusion Kinetics of Tea in Hot Water

- Diffusion is the spontaneous movement of solutes from high to low concentration
- Fick's Second Law describes how the concentration of a substance changes over time and space:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

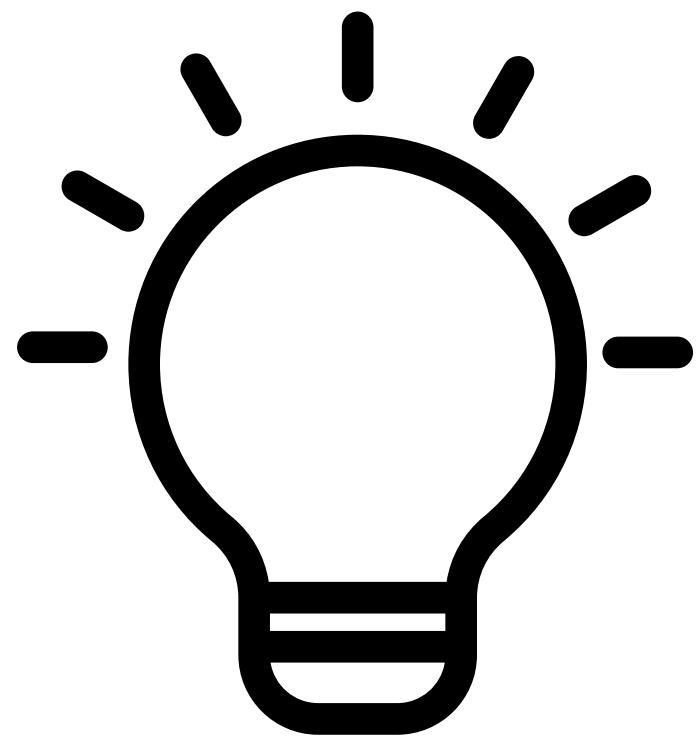
(where C is the concentration, D is the diffusion coefficient, x is the spatial coordinate (distance from the center of the tea bag), and t is time)

- In this project, we characterize the kinetics of tea extraction by tracking the absorbance of a tea solution over time using the Beer–Lambert law.
- By fitting a diffusion-controlled release model to the data, we hoped to extract meaningful parameters—such as the effective diffusivity and rate constant—at each temperature, and then use that model to extrapolate the extraction curve out to larger time scales.

MOTIVATION & INNOVATION

Predictive control of tea brewing matters for both industry (consistent flavor, caffeine yield) and the home barista. Rather than “steep 3–5 min,” we show how a physics-based model can predict how long to brew at any temperature.

We demonstrate a low-cost, colorimeter-based method to extract diffusion parameters in real time and build a predictive model.



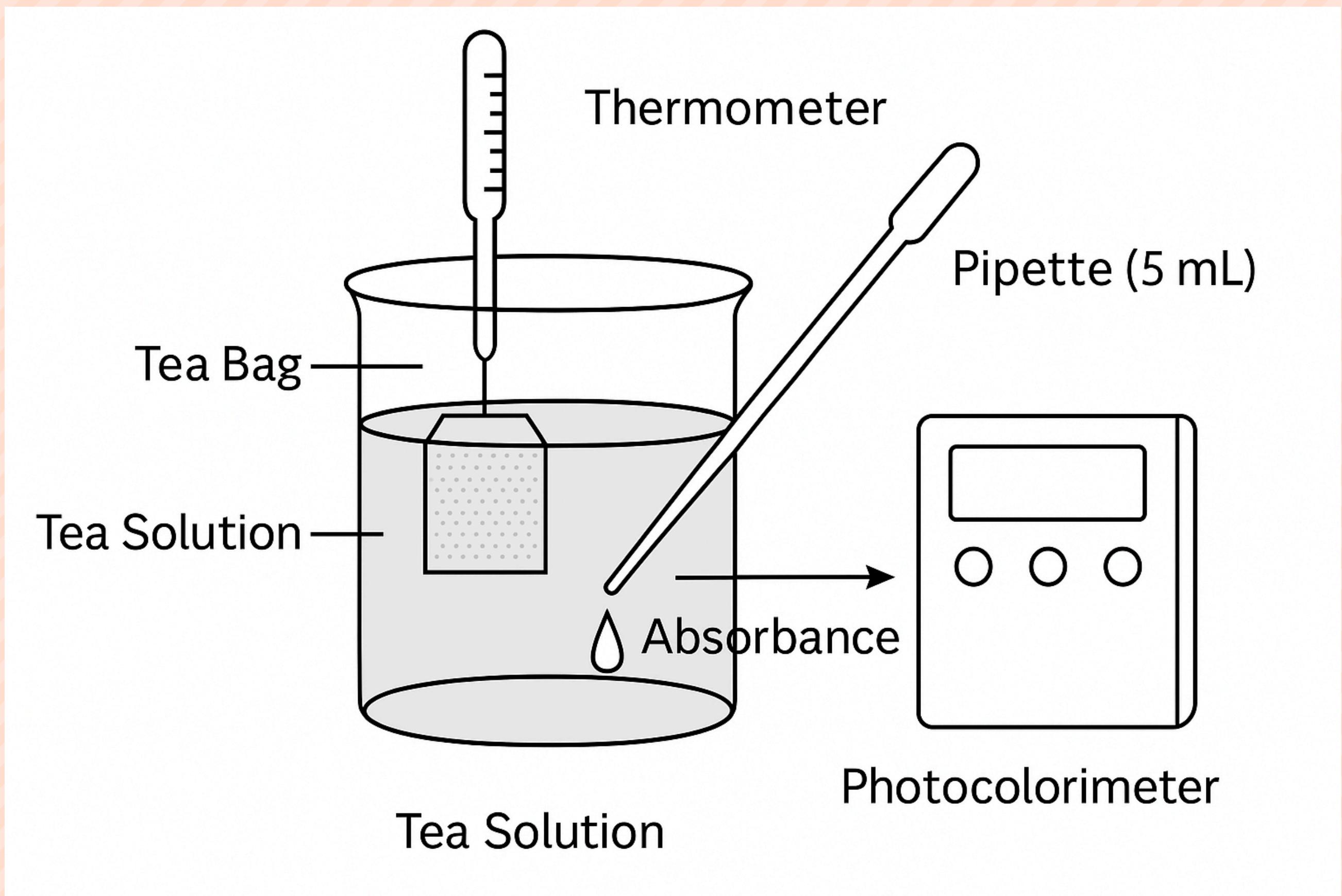
- No expensive spectrometers—just a simple lab colorimeter and open-source MATLAB.
- For future work, we can calibrate a Python programme using Computer Vision which can give us real time data just by using the images of the sample.
- We can also integrate our model into a “smart kettle” for real-time, flavor-targeted brewing.

EXPERIMENTAL SETUP

Materials used:

- Tea Bags: Each containing 2g of tea leaves.
- Water: 150 mL per trial at temperatures of 53°C, 63°C, and 73°C.
- Photocolorimeter: Measures absorbance at wavelengths between 500 nm and 550 nm.
- Pipette (5 mL): For precise sampling.
- Thermometer: To monitor and maintain water temperature.
- Beaker: To hold the water and tea bag.
- MATLAB: For data analysis and curve fitting.

DIAGRAM OF SETUP



PROCEDURE

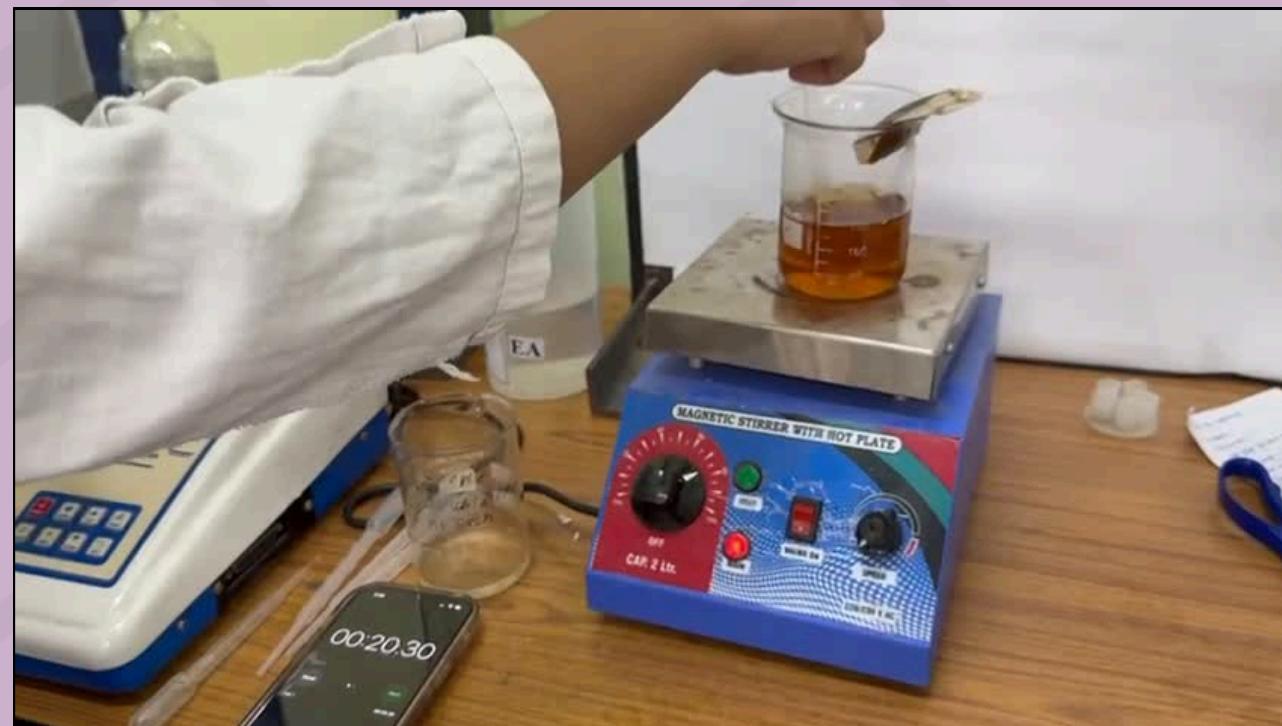
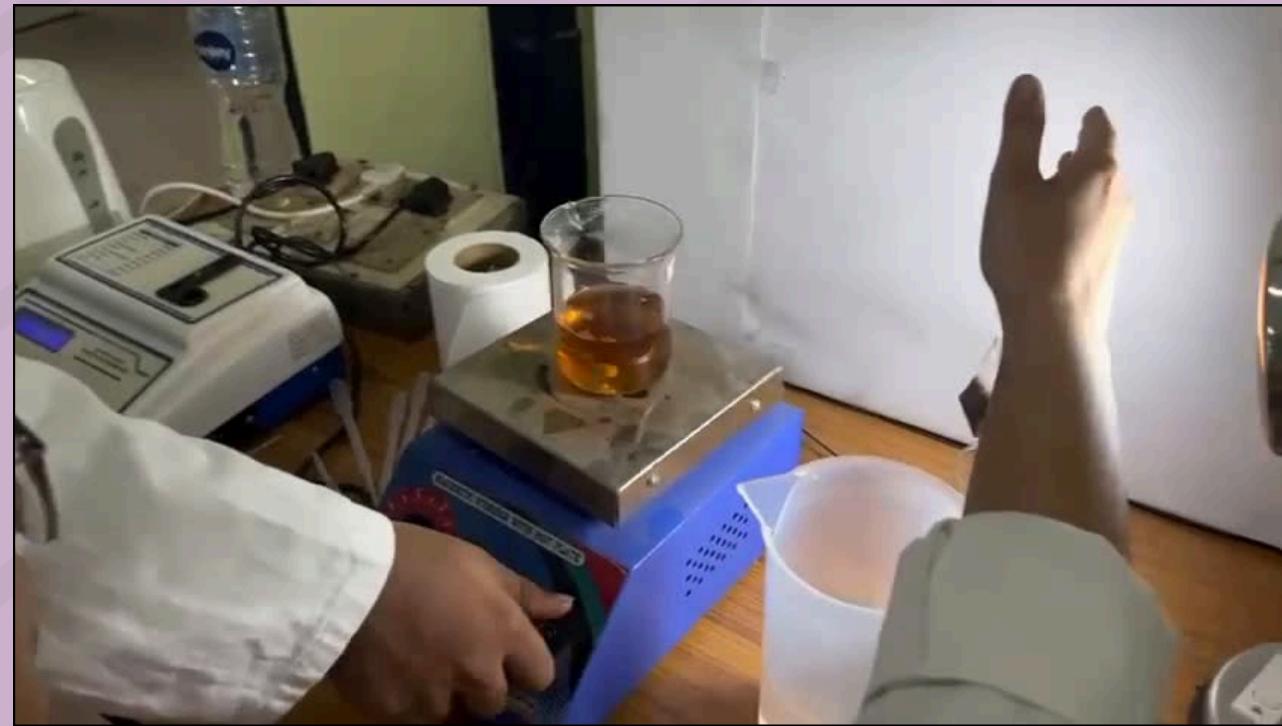
- Heat the water to the target temperature (53°C, 63°C, or 73°C).
- Immerse the tea bag into the water and start the timer.
- Extract 5 mL samples at 10-second intervals for a total of 350 seconds.
- Measure the absorbance of each sample using the photometer.
- Plot absorbance vs. time for each temperature and use MATLAB to fit the data to the diffusion model.



READINGS

Time (s)	A 53 °C	A 63 °C	A 73 °C
10	0.08	0.09	0.17
20	0.15	0.15	0.25
30	0.26	0.25	0.32
40	0.31	0.31	0.41
50	0.37	0.38	0.44
60	0.41	0.42	0.51
70	0.45	0.48	0.55
80	0.51	0.49	0.58
90	0.54	0.62	0.59
100	0.56	0.62	0.63
110	0.59	0.62	0.66
120	0.61	0.62	0.67
130	0.65	0.62	0.65
140	0.66	0.62	0.69
150	0.68	0.63	0.71
160	0.68	0.64	0.73

170	0.7	0.64	0.71
170	0.71	0.63	0.73
170	0.73	0.65	0.72
170	0.75	0.69	0.73
170	0.76	0.71	0.75
170	0.76	0.72	0.76
170	0.78	0.73	0.75
170	0.8	0.74	0.78
170	0.81	0.74	0.78
170	0.81	0.76	0.78
170	0.83	0.79	0.79
170	0.83	0.77	0.79
170	0.84	0.79	0.8
300	0.85	0.83	0.8
310	0.84	0.84	0.8
320	0.84	0.82	0.83
330	0.87	0.84	0.82
340	0.88	0.83	0.83
350	0.89	0.83	0.84
360	Nan	0.83	0.84



THEORY

System and Assumptions

To build a tractable model, we made several simplifying assumptions about how tea solute enters the bulk liquid.

- First, we treated the tea leaves themselves as contained within a roughly spherical ball of radius R , so that internal transport could be described by Fick's second law in a sphere.
- Second, with 150 mL of water stirring continuously, we assumed the surrounding fluid behaves as an infinite sink: any solute leaving the sphere disperses instantly and uniformly, so that the concentration at the sphere's surface remains effectively zero.
- Third, we neglected any resistance at the external surface of the tea-ball, assuming that internal diffusion within the leaf matrix is the rate-limiting step.
- Finally, the effective diffusivity D of solute through this porous medium was taken to be constant in time, and the initial concentration inside the sphere was assumed uniform.

Under these assumptions, Crank's classic solution for diffusion-controlled release from a sphere gives the fractional release:

$$M(t)/M_\infty = 1 - \left(\frac{6}{\pi^2}\right) \sum_{n=1}^{\infty} \left[\frac{1}{n^2}\right] \exp\left(-n^2 \pi^2 D t / R^2\right)$$

where $M(t)$ is the mass released by time t , M_∞ is the long-time plateau mass, and D is the effective diffusivity. Because the higher-order terms ($n \geq 2$) decay very quickly, a one-term approximation accurately describes the kinetics for all $t > 0$:

$$M(t)/M_\infty \approx 1 - \left(\frac{6}{\pi^2}\right) \exp\left(-\pi^2 D t / R^2\right)$$

By invoking the Beer–Lambert law (A proportional to M/V), we obtain the working absorbance model:

$$A(t) = A_\infty [1 - \left(\frac{6}{\pi^2}\right) e^{-k t}]; \quad \text{where } k = \pi^2 D / R^2$$

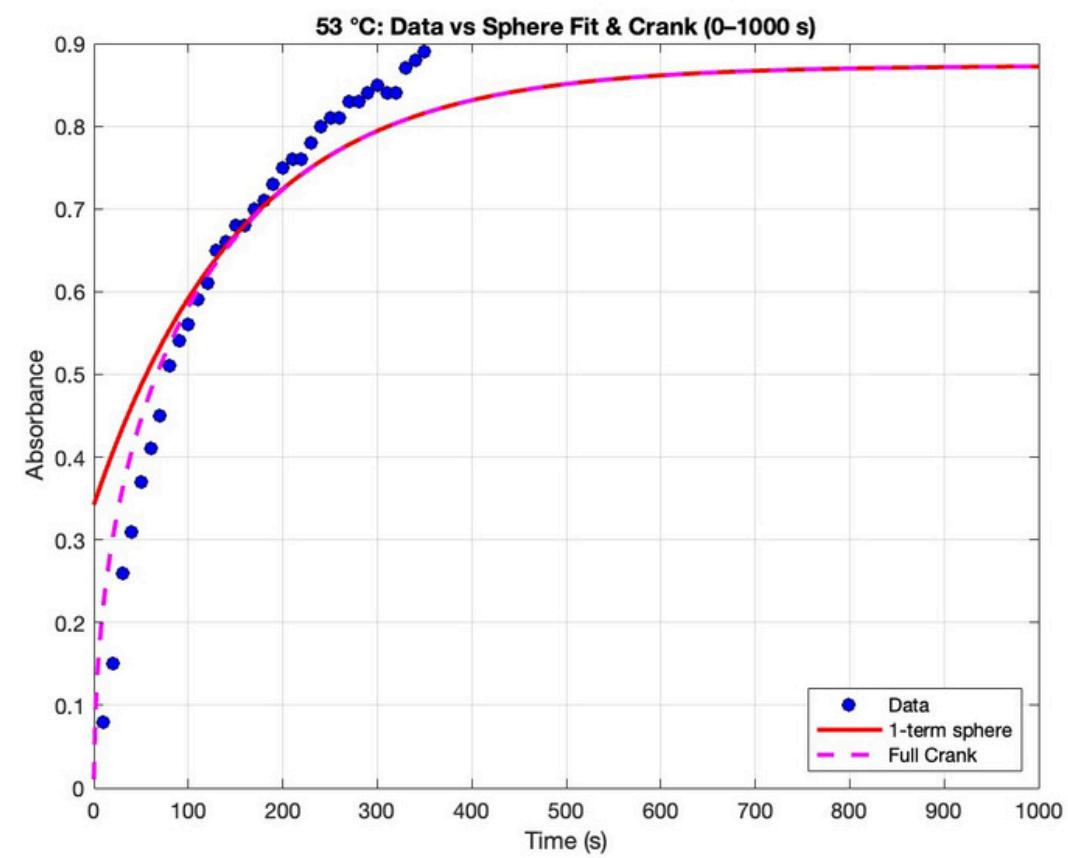
where A_∞ is the plateau absorbance and k is the effective rate constant that we will fit against our experimental data.

- D is the diffusion coefficient (how fast the tea compounds spread),
- R is the radius of the tea bag (assumed to be about 1 cm).

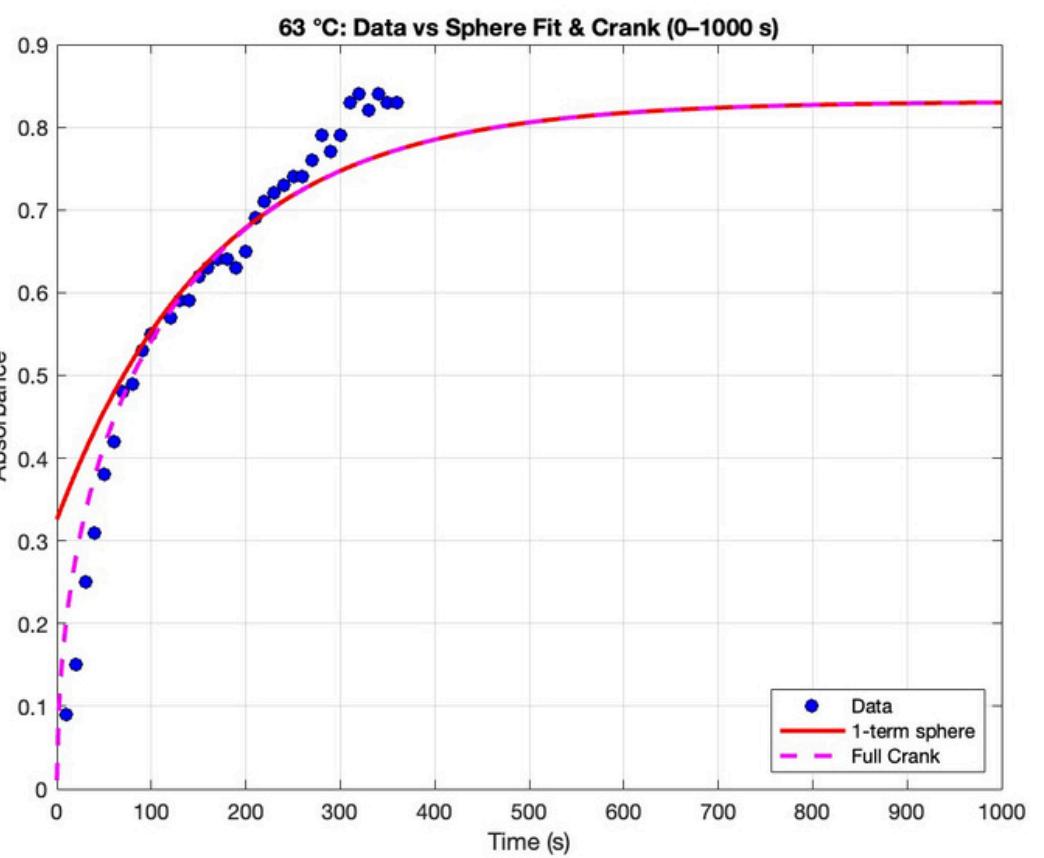
This model captures the exponential nature of diffusion: rapid initial absorption, which gradually slows as the system reaches equilibrium.

RESULTS

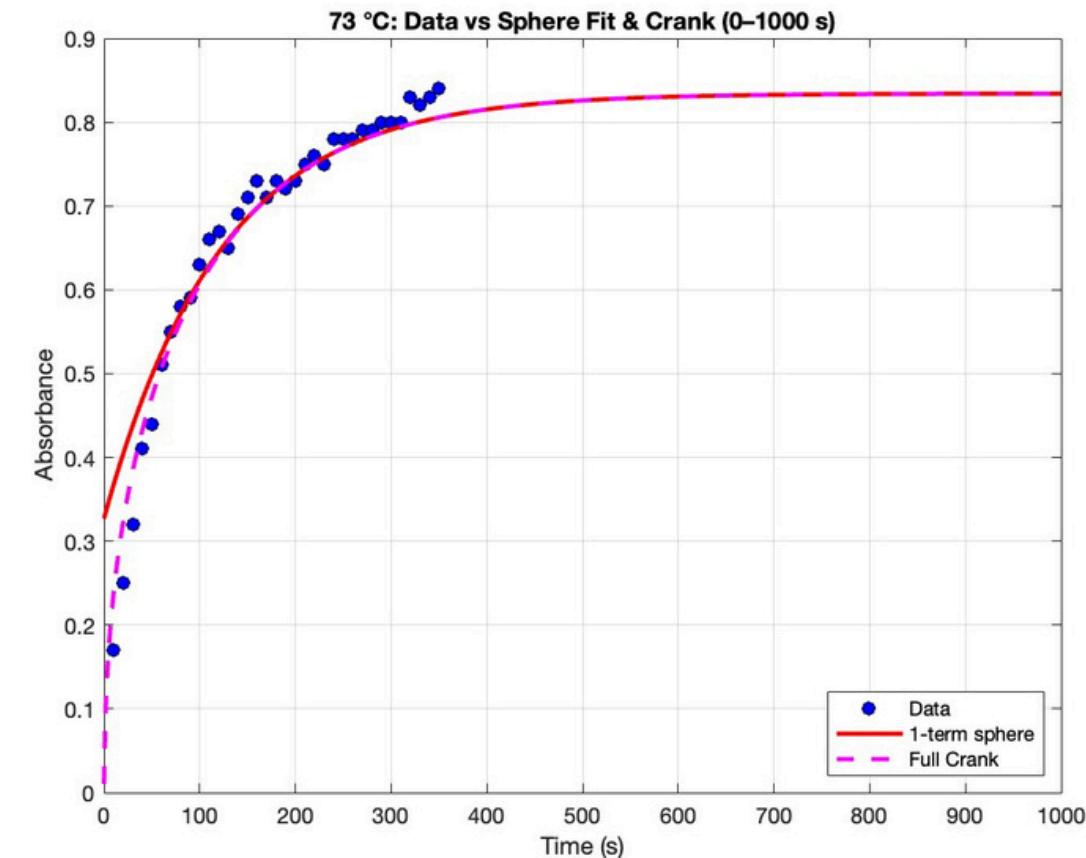
Absorbance vs Time data:



for $T=53^\circ\text{C}$



for $T=63^\circ\text{C}$



for $T=73^\circ\text{C}$

RESULTS

Calculations:

Calculations -

$T = 53^\circ\text{C}$

1) We estimate plateau absorbance A_∞ by averaging the last three readings:

$$A_\infty = \frac{A(330) + A(340) + A(350)}{3} = \frac{0.87 + 0.88 + 0.89}{3} = 0.88$$

Now, $A_f = A_\infty \left(1 - \frac{6}{\pi^2} e^{-kt}\right) \Rightarrow e^{-kt} = \frac{\pi^2}{6} \left(\frac{A_f}{A_\infty}\right)$

$$\Rightarrow k = -\frac{1}{t} \ln \left[\frac{\pi^2}{6} \left(\frac{A_f}{A_\infty}\right) \right]$$

$$\frac{\pi^2}{6} \approx 1.645$$

we find k at $t = 100, 200, 300$ sec

 $\hookrightarrow At t=100, A=0.56$

$$1 - \frac{0.56}{0.88} = 0.364$$

$$1.645 \times 0.364 = 0.599$$

$$\ln(0.599) = -0.513 \Rightarrow k_{100} = 0.00513 \text{ s}^{-1}$$

similarly for $t = 200, 300$ s $\rightarrow k_{200} = 0.00707 \text{ s}^{-1}$, $k_{300} = 0.00950 \text{ s}^{-1}$

$$k_{avg} = \frac{k_{100} + k_{200} + k_{300}}{3} \approx 0.00697 \text{ s}^{-1}$$

Now back calculating D via $D = \frac{kR^2}{\pi^2}$ ($R = 0.01\text{m}$)

$$D \approx \frac{0.00697 \times (0.01)^2}{9.8696} \approx 7.06 \times 10^{-8} \text{ m}^2/\text{s}$$

2) $T = 63^\circ\text{C}$

$$A_\infty \approx \frac{0.84 + 0.83 + 0.87}{3} = 0.853$$

$$\hookrightarrow k_{100} = 0.00581 \text{ s}^{-1}$$

$$k_{200} = 0.00509 \text{ s}^{-1}$$

$$k_{300} = 0.004819 \text{ s}^{-1}$$

$$\left. \begin{array}{l} k_{avg} = 0.00576 \text{ s}^{-1} \\ \text{(close to fitted } 0.00598 \text{ s}^{-1}) \end{array} \right\}$$

Temp (°C)	k_calc (s ⁻¹)	k_theo (s ⁻¹)	D_calc (m ² /s)	D_theo (m ² /s)	Error D (%)
53	0.00697	0.006357	7.06×10^{-8}	6.44×10^{-8}	9.61
63	0.00636	0.005983	6.44×10^{-8}	6.06×10^{-8}	6.23
73	0.00891	0.008205	9.03×10^{-8}	8.31×10^{-8}	8.62

3) $T = 73^\circ\text{C}$

$$A_\infty = \frac{0.82 + 0.83 + 0.87}{3} = 0.850$$

$$k_{100} = 0.00924 \text{ s}^{-1}$$

$$k_{200} = 0.00807 \text{ s}^{-1}$$

$$k_{300} = 0.00791 \text{ s}^{-1}$$

$$\left. \begin{array}{l} k_{avg} = 0.00891 \text{ s}^{-1} \\ \text{(highly close to fitted } 0.00821 \text{ s}^{-1}) \end{array} \right\}$$

$$D = \frac{0.00891 \times (0.01)^2}{9.8696} \approx 9.03 \times 10^{-8} \text{ m}^2/\text{s}$$

(close to fitted $8.31 \times 10^{-8} \text{ m}^2/\text{s}$)

Key observations:

- Temperature dependence: Both the hand-calculated rate constant k and diffusivity D increase with temperature, confirming faster extraction at higher temperatures.
- Agreement within 10%: The percentage error in D remains below 10% across all three temperatures. This level of agreement is excellent given the simplicity of the three-point hand method.
- Error variations:
 - At 53 °C, the 9.6% error is the largest, reflecting the slower kinetics and greater sensitivity to small uncertainties in the late-time absorbance.
 - At 63 °C, the error drops to 6.2% because the plateau is more clearly defined, making the three-point estimate more robust.
 - At 73 °C, the error rises slightly to 8.6%, as very rapid early-time extraction amplifies any timing or reading imprecision.

OBSERVATION

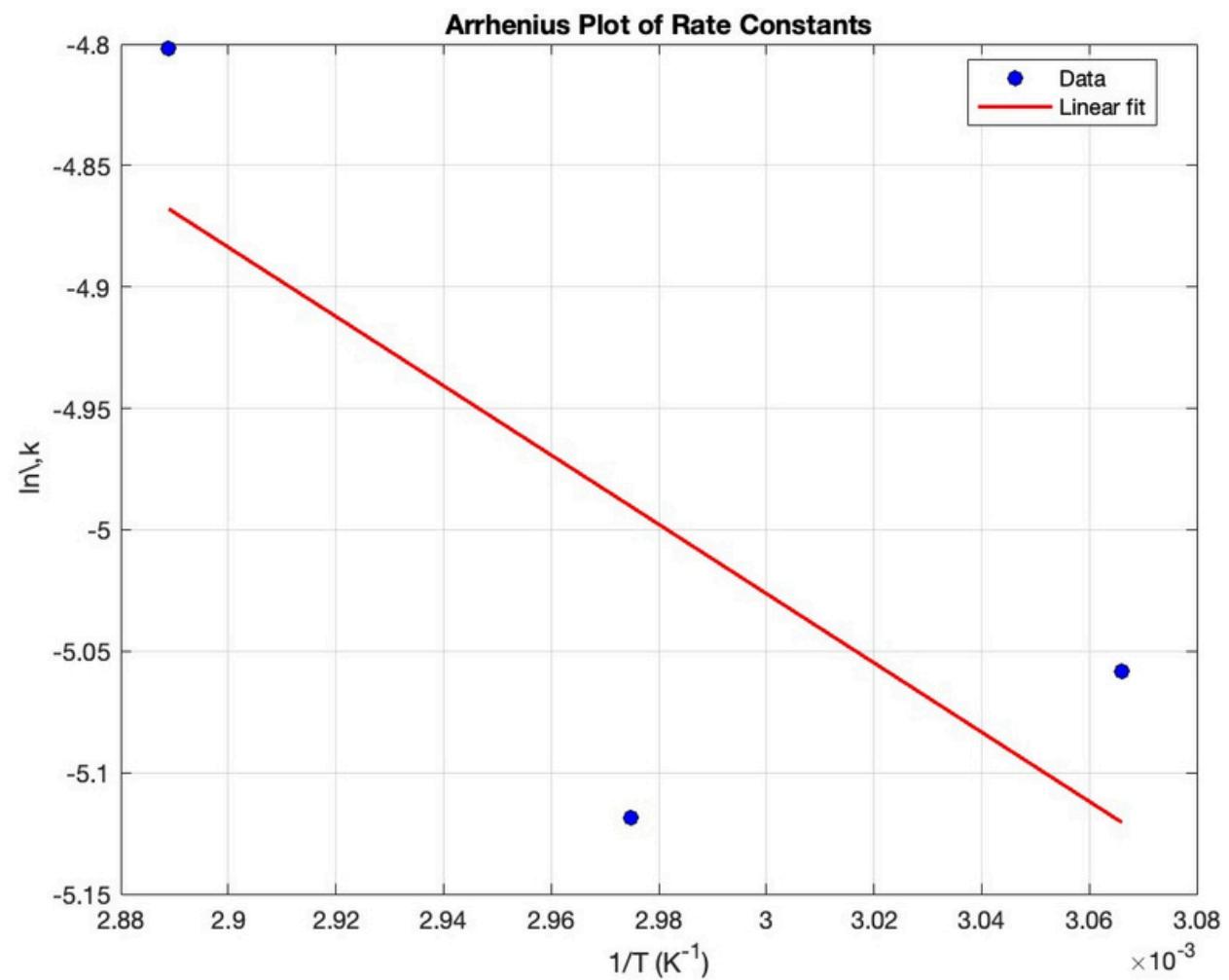
Temp (°C)	Plateau A_\infty	Rate k (s^{-1})	Diffusivity D (m^2/s)	Fit R^2
53	0.873	0.00636	6.44×10^{-8}	0.824
63	0.831	0.00598	6.06×10^{-8}	0.836
73	0.834	0.00821	8.31×10^{-8}	0.906

Key observations:

- Plateau absorbance A_∞ is similar (~0.83–0.87) across T, showing the same total extractable mass.
- Effective diffusivity D mirrors k, confirming temperature-accelerated transport.
- Fit quality R^2 improves at higher T (73 °C), since the plateau is reached earlier and noise is proportionally smaller.



INFERENCE



Our extraction rates follow Arrhenius behavior—plotting $\ln k$ vs. $1/T$ gives a straight line, letting us determine the activation energy E_a . Practically, the model predicts >95 % extraction in ~300 s at 73 °C versus ~500 s at 53 °C.

The one-term approximation and full Crank solution overlap almost perfectly, and all fits exceed $R^2=0.82$. Minor discrepancies near the plateau (<5 % of total change) stem from instrument drift, slight non-linear absorbance effects, and boundary-layer formation; adding a small film-resistance term or baseline correction would refine the late-time fit.

For future work, we can calibrate a Python programme using Computer Vision which can give us real time data just by using the images of the sample

SUMMARY

The experiment combines photocalorimetry with MATLAB-based modeling to extract important diffusion parameters like the diffusion coefficient D and the rate constant k. By applying the Beer-Lambert Law and Crank's diffusion model, we can analyze the rate of tea diffusion at different temperatures, which is expected to increase with higher temperatures.

THANK YOU

Group 12