THE UNIVERSITY OF BRITISH COLUMBIA

MURC MULTIDISCIPLINARY UNDERGRADUATE RESEARCH CONFERENCE

Modelling Diffusion in a Physically Constrained System a Numerical Approacch

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Program: Science One

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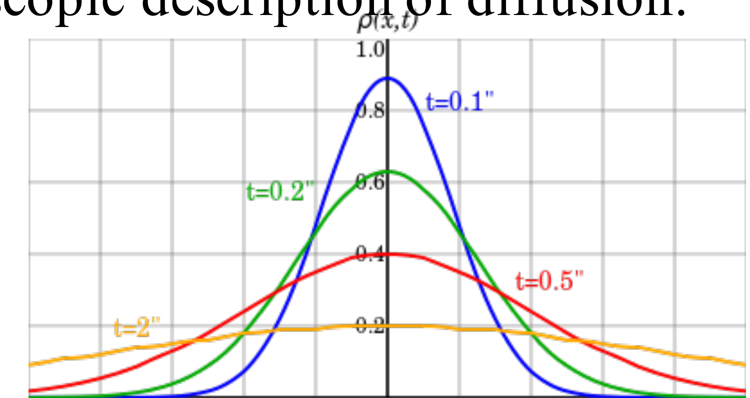
Macroscopic Diffusion: Fick's Laws

- -1855 Adolf Fick provided a macroscopic description of diffusion.
- -Fick's first law:

$$J = -D\frac{dC}{dx}$$



-Fick's second law:

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

-Diffusion occurs in the direction of a decreasing concentration gradient

-Magnitude of diffusive flux is proportional to the diffusion constant and the size of the concentration gradient.

Microscopic Diffusion: Probabilistic Collision of Particles

- -In 1905 Einstein explained the Brownian motion - stochastic movement of solute particles – is a result of the random collisions between solute and solvent particles
- -Provided evidence for the existence of atoms and a stochastic view of individual particle behaviour
- -Two key implications arise:
  - -Individual particles have an equal probability of moving in any one direction
  - -Particle movements along an arbitrary coordinate axis are independent of movements in the other axes

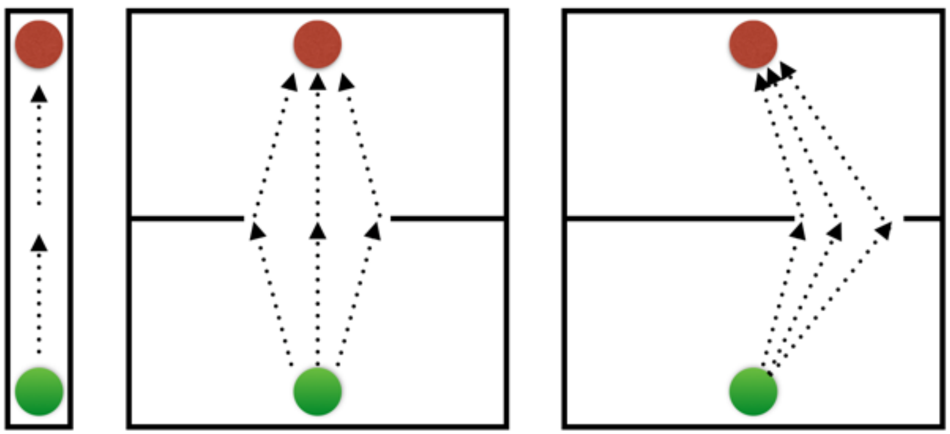
Experimental Purpose

- -Fick’s laws are limited to idealized physical systems, such as infinite and finite planes, cylinders, and cubes.
- -This study develops a mathematical model of diffusion that incorporates both the microscopic and macroscopic properties of diffusion in order to effectively model diffusion in a geometrically constrained two dimensional system.
- -Model utilizes numerical techniques.
- -Examines the feasibility of developing a more holistic model.

Basis for the Model

-A solution to Fick's second law modelling an idealized one dimensional system of diffusion is used as the basis for this study's model.

-Where, A is a dimension-less pre-exponential factor, t is time in (s), r is displacement in (m).

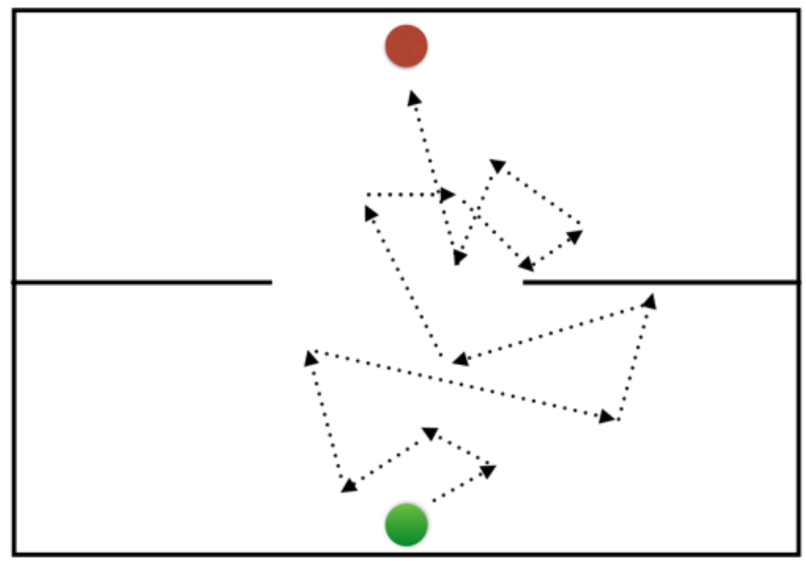


$$C(r,t) = \frac{A}{\sqrt{t}} e^{\frac{-r^2}{4Dt}}$$

The New Model's Assumptions

-The new model of diffusion treats a two dimensional diffusion process as a summation of all possible and reasonable paths of diffusion.

-A reasonable path of diffusion is defined as a path with as few directional changes as possible, and whereby all paths contain the same number of directional changes with the exception of a few more direct paths.



Angular Proportionality

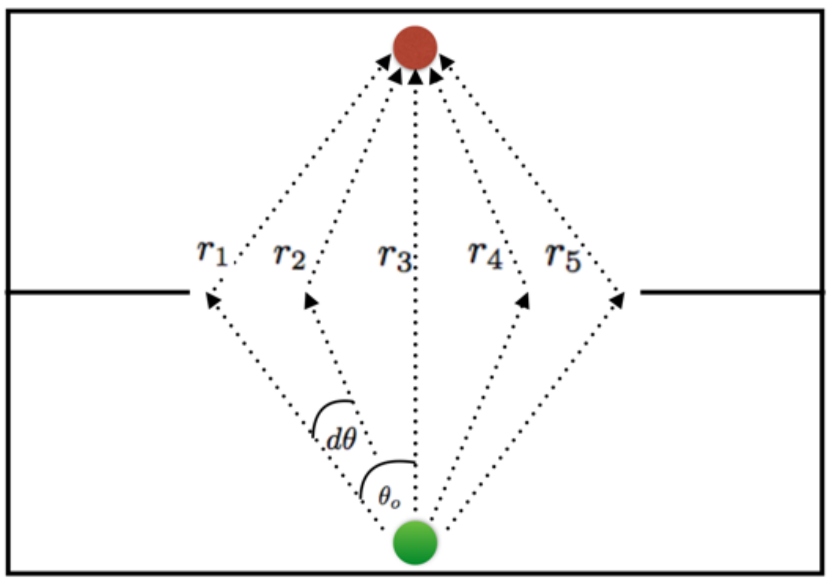
- -According to the microscopic properties of diffusion, diffusion occurs equally in any direction.
- -Thus, in a two dimensional system, each path of diffusion must contain the same amount of particles moving through it, and thus, each path should be equally spaced with respect to a central angle.

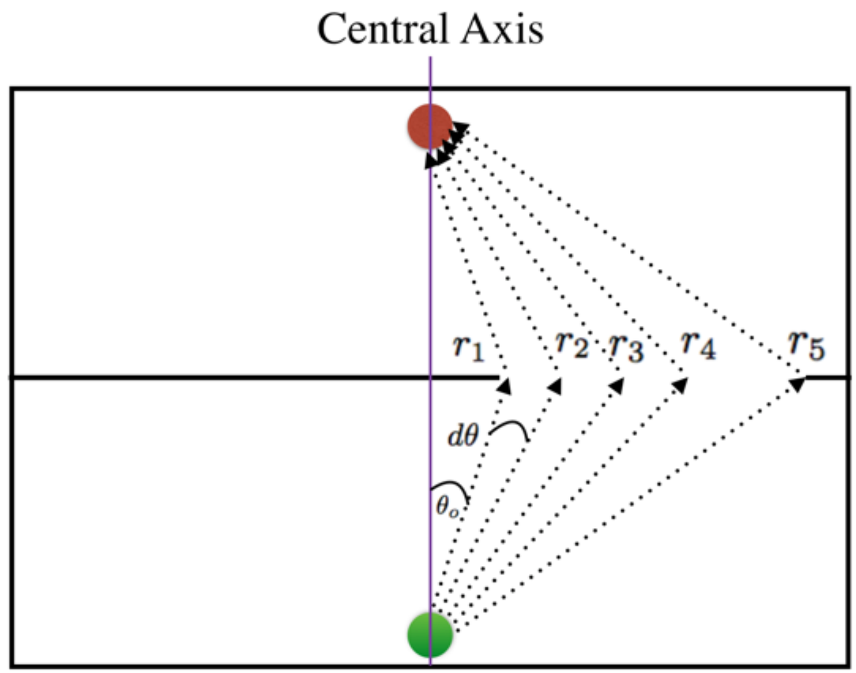
$$C(r,t) = \sum_{i=0}^{N} d\theta \times \frac{A}{\sqrt{t}} e^{\left(\frac{-(r_i)^2}{4Dt}\right)} \qquad N = \frac{\theta}{d\theta}$$

- As r_i is iterated with respect to a central angle, some function R is developed to solve this iterative solution.

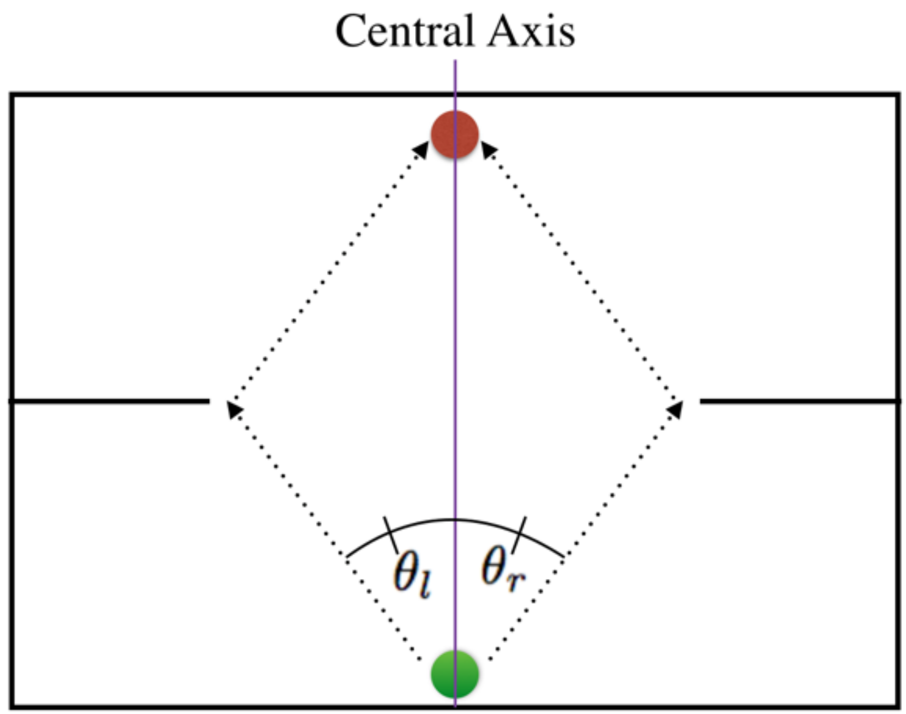
$$r_i = R(\theta_o + d\theta \times i)$$

Path of the Models





Experimental Procedure



Experimental Procedure Cont'd

To determine the effects of different slit widths and distances from the point of diffusion, the widths of the slit and the angl that the slit's edges make with the bisecting axis of the arena were varied as shown

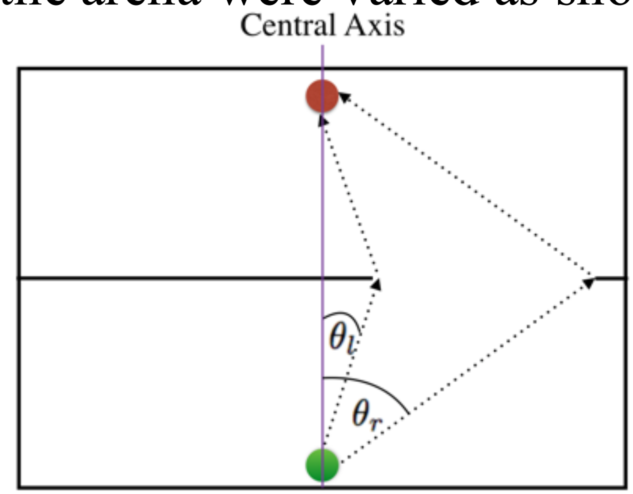


Table 1: *List of experimental treatments and their angular and dimensional parameters*

Treatment	Slit Size (cm)	Angles between Slit Edges and Axis θ_l and θ_r (degrees)
1	0 cm	N/A
2	21.2 cm	41.15^o and -45.15^o
3	1.0 cm	2.25^o and -2.25^o
4	2.0 cm	4.50^o and -4.50^o
5	4.0 cm	17.48^o and -17.48^o
6	10.0 cm	21.49^o and -21.49^o
7	2.0 cm	15.00^o and 23.05^o
8	2.0 cm	35.00^o and 40.62^o

Analyzing the Results

-For each treatment, a weighted least square fit was performed for the pre-exponential factor A in order to fit the model function to the data

-The standard deviation in pH (or concentration) at each time step between the trials in each treatment was used as the uncertainty for the fitting

-All fitted functions resulted in a p-value greater than the threshold of 0.05, implying good correlation between the model and the data

-For each experimental condition, an average pre-exponential factor was deterimed as well as the standard deviation.

-This provides an average model for each experimental condition.

Results

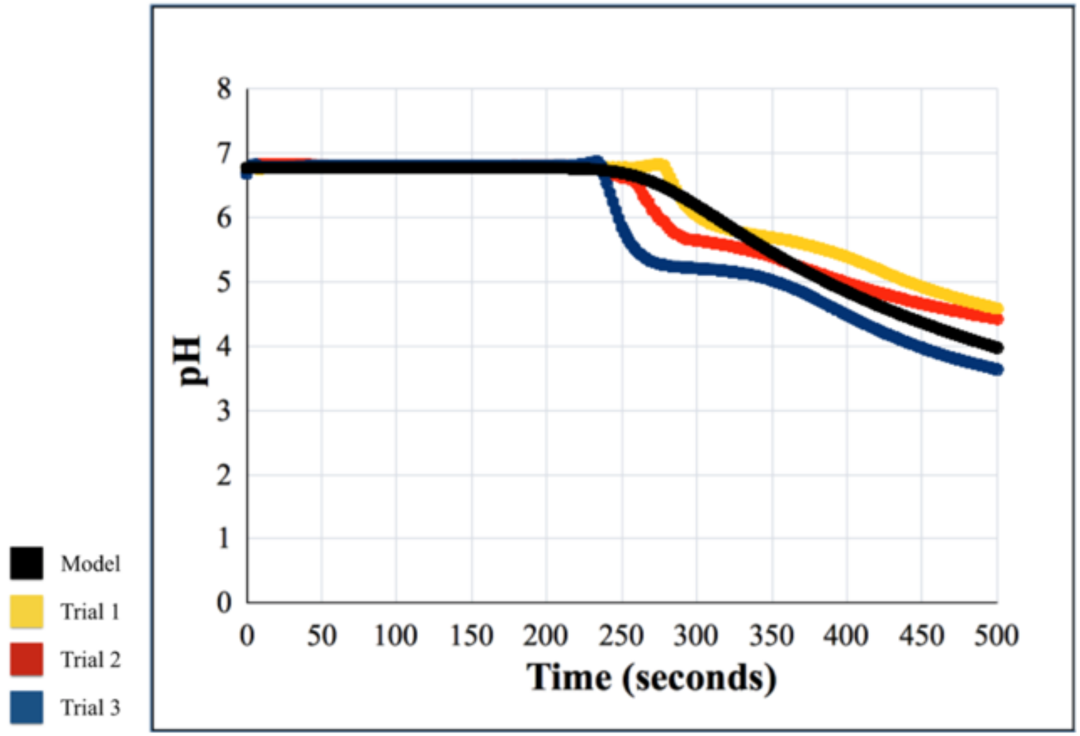


Figure 9: *Plot of continuous pH measurements in two second time intervals in the direct 1.0 cm barrier-slit treatment with the average fitted model for the treatment.*

Results

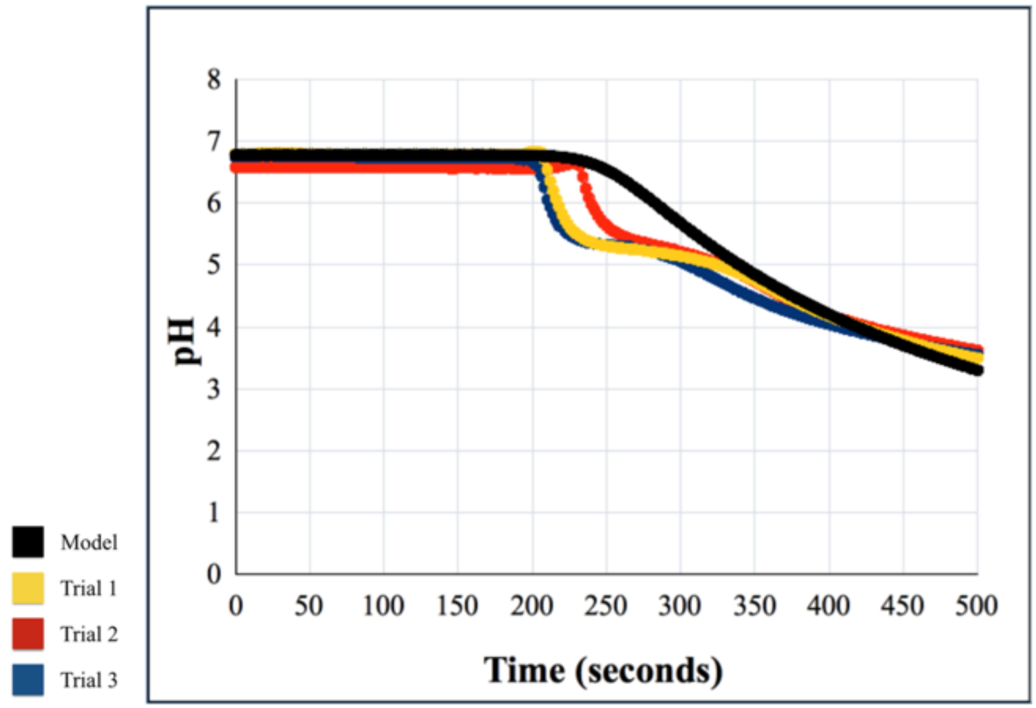


Figure 12: *Plot of continuous pH measurements in two second time intervals in the direct 10.0 cm barrier-slit treatment with the average fitted model for the treatment.*

Results

-The pre-exponential factors for all treatments were tabulated and by computing t-scores they are statistically similar

-The average A value is 3.9 ± 1.0

Table 2: *Mean A values of fitted model functions to the measurements, with standard deviations*

Treatment	A	dA
(**1**) 0 cm (no slit)	N/A	N/A
(**2**) 21.2 cm (no barrier)	5.0	1.4
(**3**) 1.0 cm slit	4.3	3.5
(**4**) 2.0 cm slit	4.1	3.0
(**5**) 4.0 cm slit	3.3	1.2
(**6**) 10.0 cm slit	3.7	0.6
(**7**) 2.0 cm slit, 15.00^o shift	3.5	1.7
(**8**) 2.0 cm slit, 35^o shift	4.5	1.7
Average	3.9	1.0

Discussion

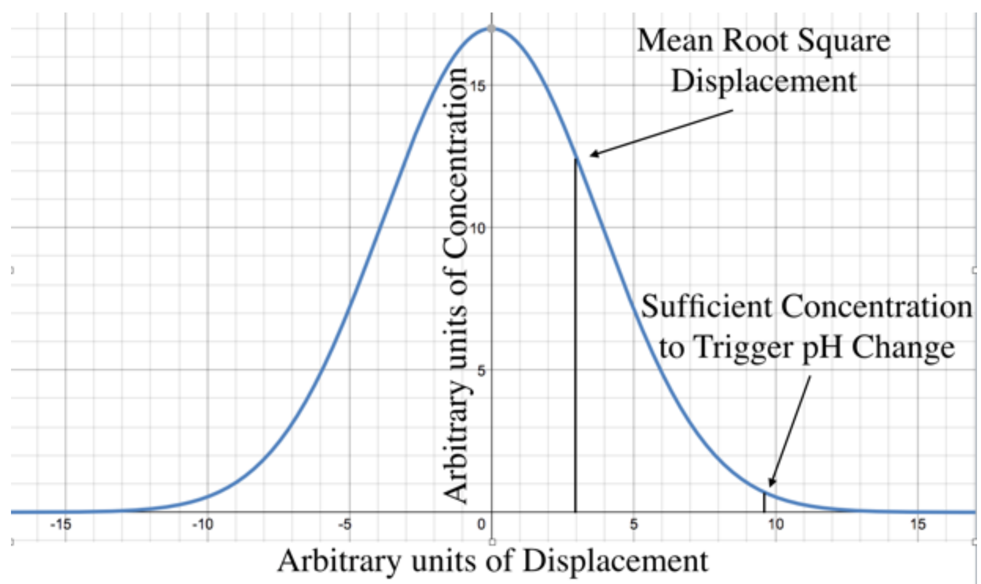
- -The T-scores between any two A values are below the theoretical threshold of 1
- -The statistically similar A values determined is in agreement with pre-established theory, implying agreement between the model and the data
- -However, this is partly due to large uncertainties which may have been due to systematic errors in the pH probe, or due to chance
- -This simplified model does not take into account limitations of the experimental setup
  - Reflection
  - The "point" of insertion is not truly just a point

Discussion: Theoretical Discrepancy

- -An apparent contradiction: Using the mean root square approximation, the average distance displaced by a diffusing hydronium particle in 500 seconds is less than 2 mm!

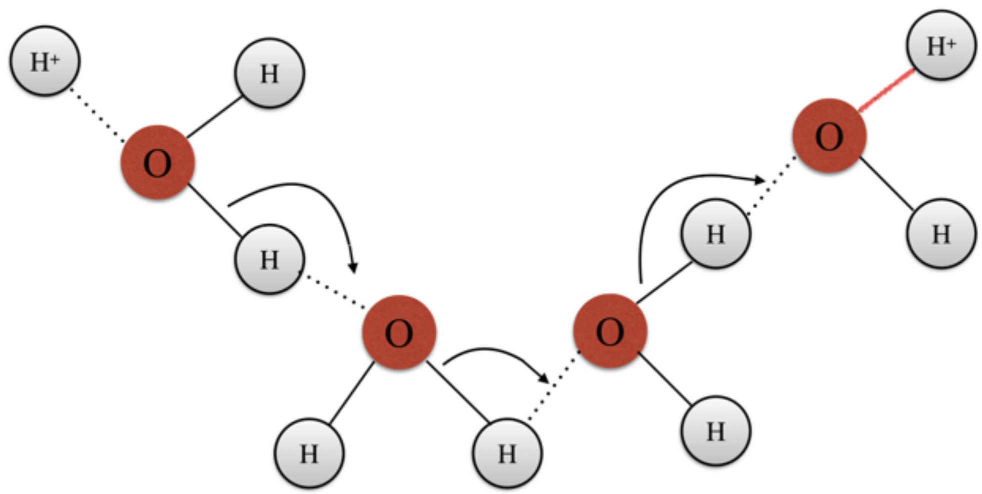
-This could be justified by considering that this is only the mean root square displacement, not the maximum distance travelled by any particle

-Presence of less than 0.01% of the total hydronium ions added could trigger a pH change from 7-5



Discussion: Other Explanations

-Other possible factors for this apparent discrepancy include the diffusion of charge by the rapid breaking and forming of O-H bonds in water and hydronium molecules.



-Alternatively, the transfer and opening of the acid container could have caused the hydronium particles to have an initial velocity

Conclusion

- Pre-exponential factor A remains roughly constant at 3.9 ± 1.0, consistent with theoretical expectations, shows that the model accounts for the physical system without required correction.
- Implies that this numerical approach can be applied to more complex systems, and more research should be performed on developing such a model.
- Any enclosed physical system could potentially be modelled using this approach, with applications in industrial settings

References

- Fick A, On liquid diffusion. *Journal of Membrane Science*. **1995**, 100, 33-38
- Einstein, A. *Investigations on the theory of Brownian Movement*; Dover Publications: New York, 1956
- Edward, J.T. Molecular Volumes and the Stoke-Einstein Equitation. *Journal of Chemical Education*. ***1970.*** *47(4), 261-169*
- *Crank, J. The Mathematics of Diffusion*, 2nd ed.; Oxford University Press: London, 1975.
- Haynes W.M. *CRC Handbook of Chemistry and Physics,* 96th Edition (Internet Version.; CRC Press/Talor and Francis: Bocas Raton, FL, **2016**)

Acknowledgements

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