

Modeling Diffusion Rates of a Gas in an Enclosed Space

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Abstract: This research attempts to identify the relationship between pressure of a certain gas and diffusive flux in a closed system by 1) creating a mathematical model and 2) constructing a physical apparatus to test the model in the real world. Using Fick's Law as a basis for the calculations, a differential equation was used to discern an ideal, theorized relationship between the two parameters. This relationship is shown below.

$$\frac{dX}{dt} = \frac{AD}{L} * P * e^{-d * \frac{V_2 + V_3}{V_2 * V_3} * t},$$

where A, D, L, t, V_2 and V_3 are all constants.

The experimental findings suggested a similar linear relationship, $y = 10.186x - 1179.1$ where y represents the rate of diffusion of CO₂ and x represents the pressure of the CO₂. Thus, the theoretical hypothesis holds consistent with the experimental findings, implying a linear correlation between pressure of a gas and rate of diffusion.

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Introduction:

The purpose of this research project was to identify a relationship between pressure and diffusive flux between two gases in a closed system. We took two-pronged approach to this question: mathematically and experimentally. We then decided to compare the two results, for further justification. Mathematically, we applied Fick's first law in one-dimension as well as the Ideal Gas Law, and we solved the associated first-order differential equation to obtain a formula for the distribution of gas at any moment. We then differentiated this formula to generate an expression for the diffusive flux as a function of the initial pressure and time.

Experimentally, we constructed a physical apparatus designed to test this result. The test apparatus has two chambers, one filled with air and the other filled with pure carbon dioxide. When we connected these two chambers, we allowed the carbon dioxide gas to diffuse to the ambient air chamber and measured the diffusion rate through a carbon dioxide sensor, and then we divided by the cross-section area of our apparatus to obtain the diffusive flux. We then compared the computed diffusive flux with the measured diffusive flux.

Mathematical Theory

We use Fick's law shown below as the basis for our result.

$$\frac{dN_{CO_2_3}}{dt} \cdot \frac{1}{A} = \frac{P_2 - P_3}{L} \cdot D$$

$N_{CO_2_3}$:= the amount of carbon dioxide particles in chamber 3

P_3 := the pressure of carbon dioxide in container 3

P_2 := the pressure of carbon dioxide in container 2

A := the cross-sectional area of connection between the two containers

D := the diffusion constant

Rewrite the $N_{CO_2_2}$ in terms of N and $N_{CO_2_3}$ using the ideal gas law (Recall $PV = nRT$)

$$\frac{dN_{CO_2_3}}{dt} \cdot \frac{1}{A} = \frac{\frac{(N - N_{CO_2_3}) \cdot RT}{V_2} - \frac{N_{CO_2_3} \cdot RT}{V_3}}{L} \cdot D$$

$N_{CO_2_2}$:= the amount of carbon dioxide particles in chamber 2

R := ideal gas constant

V_3 := Volume of container 3

V_2 := Volume of container 2

T := Temperature

N := the total number of carbon dioxide particles in the system ($N_{CO_2_3} + N_{CO_2_2}$)

Let:

$$x = N_{CO_2_3}$$

$$d = \frac{ADRT}{L}$$

Substitute the values

$$\frac{dx}{dt} = d \cdot \left(\frac{N}{V_2} - \frac{V_2 + V_3}{V_2 V_3} x \right)$$

Use separation of variables to solve the homogeneous first order linear differential equation for the amount of carbon dioxide.

$$x = ce^{-d \frac{V_2 + V_3}{V_2 V_3} t} + \frac{V_3}{V_2 + V_3} N$$

Plug in the initial state ($x(0) = 0$)

$$c = -\frac{V_3}{V_2 + V_3} N$$

Plug in c

$$x = -\frac{V_3}{V_2 + V_3} N e^{-d \frac{V_2 + V_3}{V_2 V_3} t} + \frac{V_3}{V_2 + V_3} N$$

Differentiate both sides in order to find the function of the pressure gradient with respect to P:

$$\frac{dx}{dt} = N \left(-\frac{V_3}{V_2 + V_3} \cdot -d \frac{V_2 + V_3}{V_2 V_3} \right) e^{-d \frac{V_2 + V_3}{V_2 V_3} t}$$

Use the ideal gas law to substitute N for P :

$$\frac{dx}{dt} = \frac{PV_2}{RT} \left(-\frac{V_3}{V_2 + V_3} \cdot -d \frac{V_2 + V_3}{V_2 V_3} \right) e^{-d \frac{V_2 + V_3}{V_2 V_3} t}$$

Simplify (Recall $d = \frac{ADRT}{L}$):

$$\frac{dx}{dt} = \frac{AD}{L} \cdot P e^{-d \frac{V_2 + V_3}{V_2 V_3} t}$$

Plug in the experimental constants to find the formula describing our apparatus:

$$\frac{dN_{CO_2}}{dt} = 1.55 \times 10^{-7} \cdot P e^{-0.35t}$$

Experimentation:

Parts Lists:

Required Materials	Quantity	Source	Total Price
4' of 1" radius PVC pipe	3	Home Depot	10\$
PVC 1"-1.5" Adapter	1	Home Depot	1.5\$
6.5" of 1.5" radius PVC pipe	1	Home Depot	3.65\$
PVC cement	1 Set	Borrowed from SSA Robotics Lab	N/A
1" radius ball valves	2	Home Depot	10.58\$
Vacuum Pump	1	Borrowed from SSA Science Lab	N/A
1" radius couplings	2	Home Depot	1.00\$
Brass Fitting - 1/4 "	1	Home Depot	3.99\$
Brass Fitting - 3/4 "	1	Home Depot	3.99\$
Dry Ice (in Pounds)	10 (the minimum quantity for sell)	Mastro Ice Inc	15\$
Vernier Gas Pressure Sensor	1	Borrowed from SSA Science Lab	N/A
Vernier CO2 Gas Sensor	1	Borrowed from SSA Science Lab	N/A
Vernier Labquest Mini	1	Borrowed from SSA Science Lab	N/A
Computer with USB port and Logger Pro	1	Chirag's Macbook Pro	N/A

Design:

We decided to have a ball valve between each compartment so that there would only be two positions for the valves. We did this so that there would be as small time between the opening of the valve so that there would be as little error as possible. From the left to the right, first we have Chamber 1, or the dry ice chamber, with a removable end cap to facilitate the insertion of dry ice. The endcap is not completely sealed; yet because dry ice powder evaporates very fast, this turned out to be a minor problem. We then have the first valve, Valve 1, connecting two chambers. On the other side of Valve 1 is Chamber 2, the CO₂ chamber. In Chamber 2, we have two barbed fittings. The first of these barbed fittings connects to a pressure sensor, which lets us monitor the pressure while we vacuum out Chamber 2. The barb fitting that connects to the vacuum pump is also connected on this side. Then, we have Valve 2, connecting Chambers 2 and 3, which holds our ambient air. The CO₂ sensor is connected to the end of Chamber 3, to detect the amount of CO₂ that diffuses through the apparatus. From this information, we can determine the diffusion rate by taking the derivative over time of the data. Because the amount of CO₂ in ambient air is fairly constant (approximately 300 ppm), placing the CO₂ sensor on the air side allows us to capture the CO₂ change due to diffusion well. The entire system is sealed with PVC cement, teflon tape and regular tape; the sealing proves to be fairly good, allowing us to reach a pressure of 7 kPa (about 7% of atmospheric pressure) when we fully vacuum out the CO₂ chamber. A diagram of our physical system can be found below.

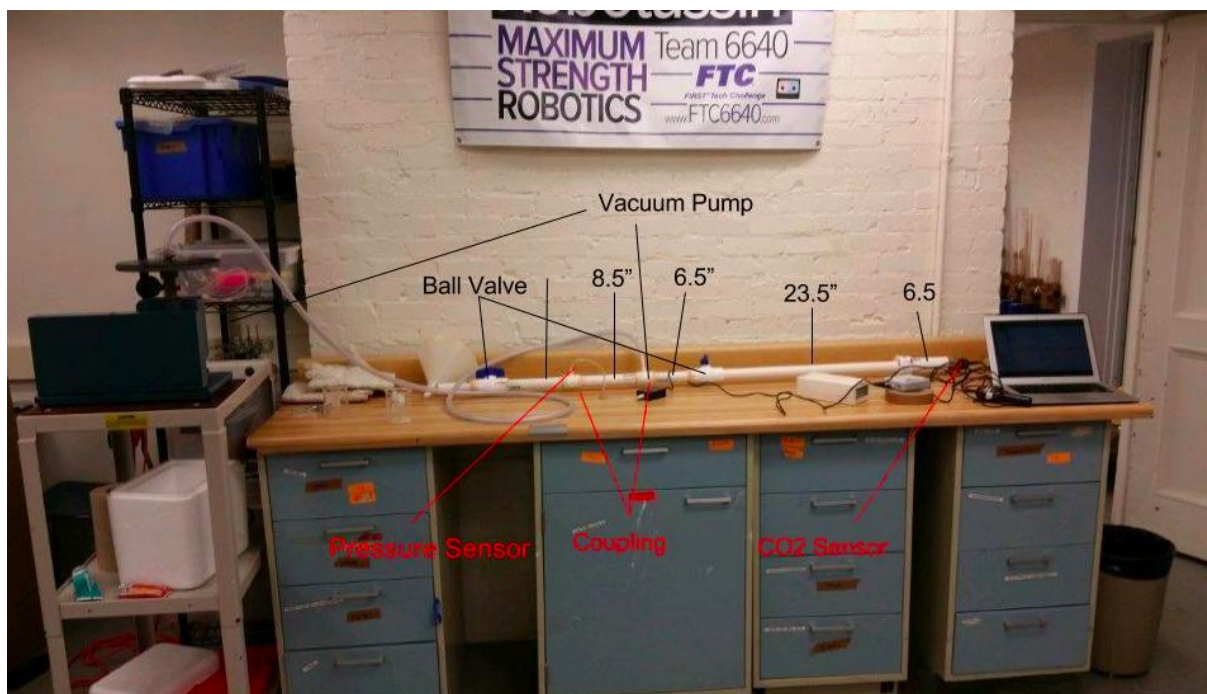


Image 1: The graphic above shows our experimental apparatus, complete with labeled parts.

Procedure:

We implemented a multi-stage plan to approach this experiment, as shown below.

Step 1: Apparatus Preparation

A) *CO₂ Loading*

We loaded our blocks of dry ice into a sink and used a hammer to break the blocks into more refined pieces. We weighed a standard, empty 500 ml Beaker (106 grams) on a scale and then poured the crushed pieces of dry ice into the beaker. We then weighed the beaker with the dry ice to obtain an accurate measurement of exactly how much dry ice, and consequently CO₂, we were loading into the gas chamber. After recording the mass, we closed all the valves of our apparatus, took off the end cap, and used a funnel to pour the dry ice into the first chamber. We immediately placed the end cap back onto the first chamber to prevent any sublimation from the dry ice outside of the chamber. Then, we waited for approximately 5-10 minutes, depending on the amount of dry ice, so that the solid could turn to its gaseous form.

B) *Vacuum Pumping*

To make sure we have as pure of a concentration of CO₂ as possible, we vacuumed the ambient air out of the second gas chamber. Ideally, we would have had a pressure of 0 kPa, but our Vacuum Pump was not powerful enough to create a pure vacuum, so we were only able to maintain a pressure of around 7 kPa. However, we decided it was a small enough amount of air that it would not affect our data too much.

Step 2: Mixture of the Gases

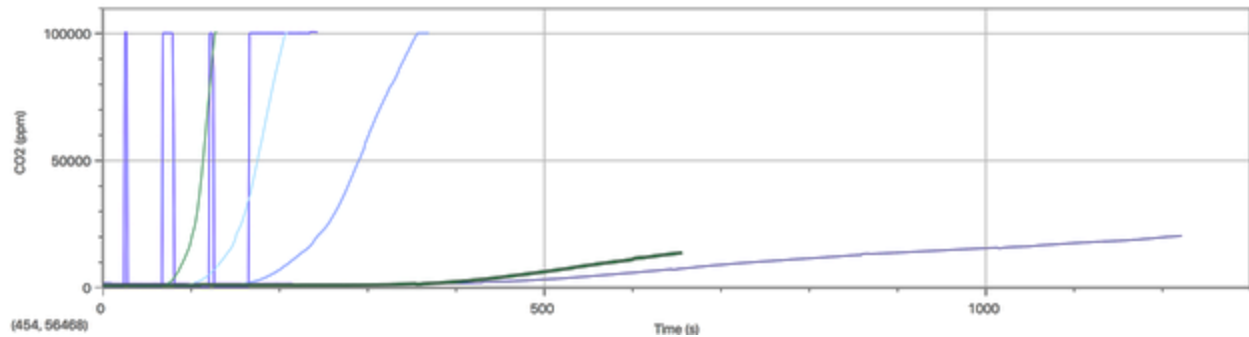
Once the dry ice has dissolved, we turn off the vacuum pump and open up the valve from Chamber one to Chamber two. The vacuum sucks in the CO₂ in gaseous form. Then, once we reach the expected, calculated pressure (measured from the pressure sensor), we open up the valve from Chamber two to Chamber three. This allows for the diffusion between CO₂ and ambient air. We start data collection at that instant.

Step 3: Post Run Cleanup

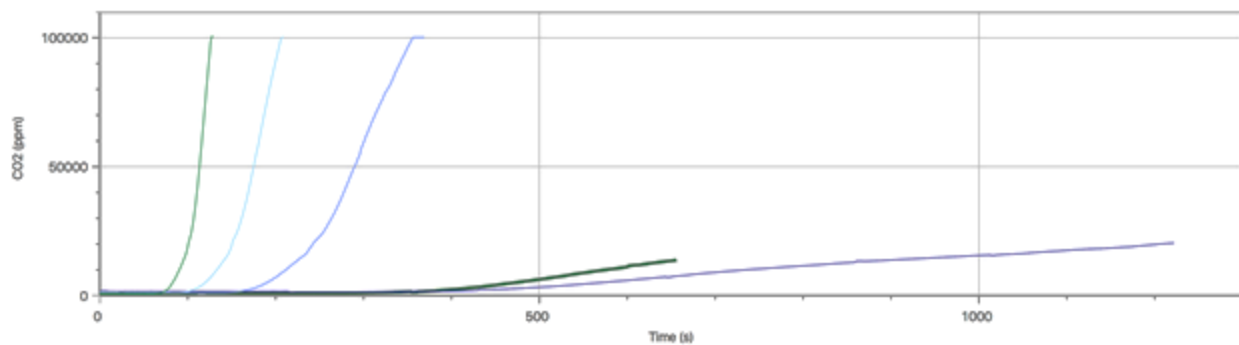
After our diffusion has run its course and we have established a stable rate, we stop the run on Logger Pro. Then, we turn the vacuum pump on to empty the tube of CO₂. We monitor the CO₂ concentration to determine when it reaches the level of that of air. Then we open up the valves and take off the end cap so the pressure can re-stabilize to room pressure (101 kPa). Now the apparatus is ready for another run.

Results:

We used Logger Pro V3.0 to synthesize all of the incoming data from the labquest CO2 sensor. Our data is shown below in two graphs, with CO2 concentration as a function of time.



Graph 1: This is a graph of CO2 concentration vs time at different masses. The first sporadic purple line is an outlier, at 6.5 grams, due to a faulty CO2 sensor. After that initial run, we changed the CO2 sensor and received much more predictable readings.



Graph 2: Above is a graph of CO2 concentration vs time at different masses, without the outlier. Legend of the graphs, from left to right: Green - 7.5 grams, Light Blue - 4.8 grams, Dark Blue - 3.0 grams, Dark Green - 2.2 grams, Purple - 1.6 grams.

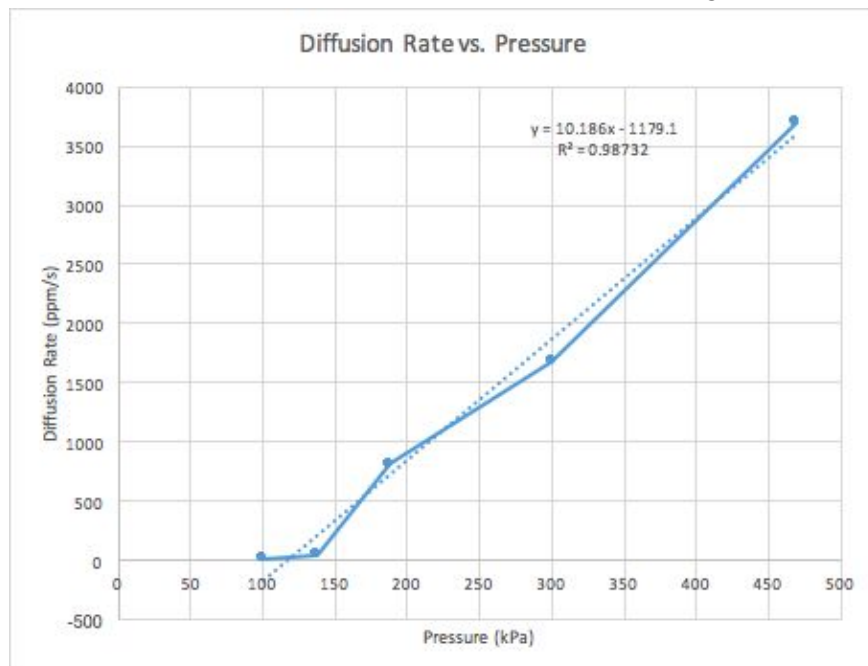
Analysis

Data Analysis

After obtaining our data, we now convert to our required metric. First, we took the derivative of each trial at the halfway point of each time window. The derivative of CO₂ concentration over time is the rate of diffusion over time. Then we converted the mass of dry ice to pressure in Chamber 2, using the ideal gas law. The converted data is shown below.

Pressure (kPa)	Diffusion Rate (ppm/s)
100.012	17.8
137.516	46.6
187.522	819.9
300.036	1683
468.807	3698

Table 1: Converted data to pressure and diffusion rate. Pressure was calculated using the ideal gas law, $P=nRT/v$, where n is the number of molecules deduced from molecular weight.



Graph 3: Plotted points from Table 1, with a linear trend line shown as well. The best fit line is a linear equation, $y = 10.186x - 1179.1$ at a correlation of 0.987.

Error Analysis

Since we put the dry ice into one side of the container, we opened the end cap and placed dry ice inside the compartment. However, when we opened the compartment we also allowed some air into the tube which would have allowed some air to come inside. When we first held our experiment we heard a whistle from the tube, and we deduced that there was some leakage in the tube. So to fix this, we pinpointed the place where we heard the whistle and covered the spot with masking tape. Then, to be sure that there was no leakage at any other connections, we covered all of the connections with masking tape. However, while we may have had some leaks which would skew the data, we did not experience any major leaks in the apparatus, because there were no changes in pressure inside the apparatus during the experiment except for the original change in pressure due to the opening of the valve. Lastly, due to the limitations of our technologies, we could not see the graph approach a stable value, because either it would take too long or the stable value was past 10,000 ppm and so it was difficult to fit data to a curve.

Conclusion

Our experimental findings were consistent with our theorized hypothesis. We predicted a linear correlation between pressure and diffusion rate of CO₂: $1.55 * 10^{-7} * P * e^{-0.35t}$, with P being pressure measured in pascals. Our experimental findings held to this prediction, with a relationship of the same form: $y = 10.186x - 1179.1$, with x being pressure measured in kPa. Though the constants may vary between our theoretical and physical system, the relationships are still of the same form. Thus, our hypothesis is correct and as pressure increases, the rate of diffusion increases at a linear rate.