Theoretical Pressure

According to the law of ideal gases,

$$PV = nRT$$

As we mentioned earlier, our container is closed and therefore the volume remains constant. Now, if we disregard changes in ambient temperature, we have:

$$\frac{P}{n} = \frac{RT}{V} = cte.$$

From here we get:

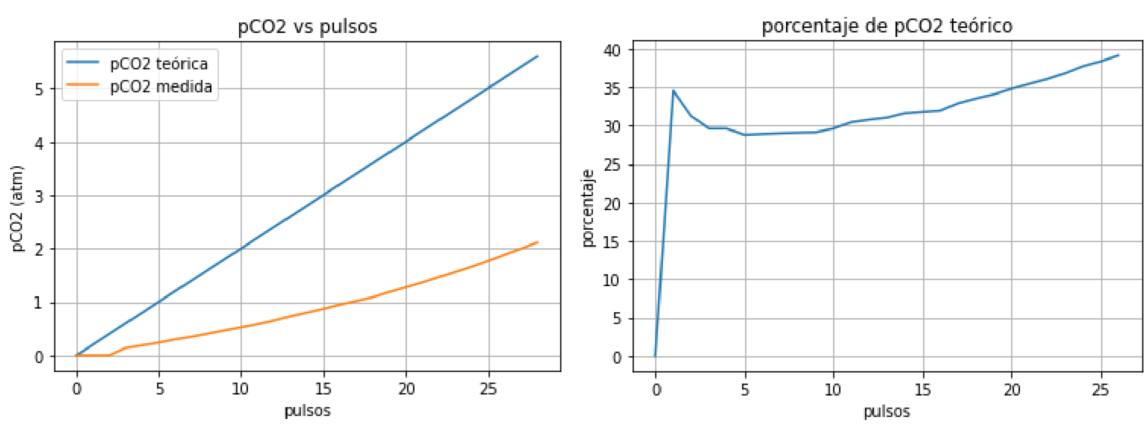
$$\frac{P_i}{n_i} = \frac{P_f}{n_f} \rightarrow P_f = P_i \frac{n_f}{n_i}$$

Avogadro's law tells us that "equal volumes of *all gases*, at the *same* temperature and pressure, *have the same number* of molecules" so we can substitute the number of particles for the volume of gases. In this way, we can calculate the theoretical partial pressure of the vessel based on the pulses that we are injecting.

$$P_f = P_i \frac{V_f}{V_i} = P_i \frac{V_{recip} + V_{CO_2}}{V_{recip}}$$

$$pCO_2 = \frac{V_{CO_2}}{V_{recip} + V_{CO_2}} P_f = \frac{V_{CO_2}}{V_{recip} + V_{CO_2}} P_i \frac{V_{recip} + V_{CO_2}}{V_{recip}} = P_i \frac{V_{CO_2}}{V_{recip}}$$

$$pCO_2 = \frac{V_{CO_2}}{V_{recip}} \; atm$$



pH and other components

Another topic of interest is to know the proportion of components in the mixture, these can be obtained through chemical equations, the development is as follows.

Carbon dioxide dissolved in water is in equilibrium with carbonic acid:

$$CO_2 + H_2O \rightleftharpoons \ H_2CO_3$$

The equilibrium constant at 25°C is K_h = 1.70×10−3: therefore, most carbon dioxide is not converted to carbonic acid and remains as CO2 molecules.

Carbonic acid is diprotic, i.e. it has two dissociating hydrogens and therefore two dissociation constants:

$$H_2CO_3 \ \rightleftharpoons \ HCO_3 - \ + H^+$$

$$K_{a1} \ = \ 2.5 \times 10^{-4} \frac{mol}{L}; \qquad pK_{a1} \ = \ 3.60 \ a \ 25\ °C.$$

$$HCO_3 - \rightleftharpoons \ CO_3{}^{2-} \ + \ H^+$$

$$K_{a2} \ = \ 5.61 \times 10^{-11} \frac{mol}{L}; \qquad pK_{a2} \ = \ 10.25 \ a \ 25\ °C.$$

The last equation to take into account is the

At constant temperature, the composition of a pure carbonic acid solution (or a pure CO2 solution) is completely determined by the partial *pCO2 pressure* of carbon dioxide on the solution. To calculate this composition, it is necessary to take into account the above equilibria between the three different forms of carbonate (*H2CO3, HCO3− and CO32−*), as well as the hydration balance between *dissolved* CO2 and *H2CO3* with constant

$$K_h = \frac{[H_2CO_3]}{[CO_2]} = \ 1{,}70 \times 10^{-3}$$

and the following balance between dissolved CO2 and gaseous CO2 on top of the solution:

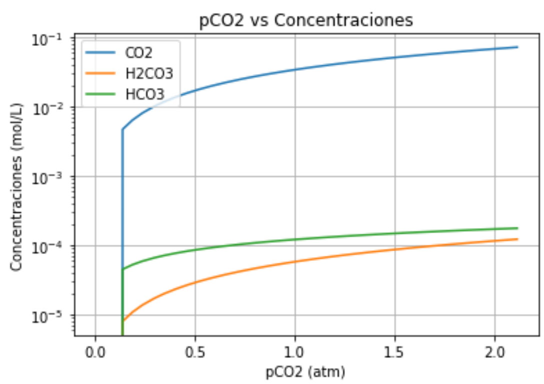
$$\frac{[CO_2]}{pCO_2} = \frac{1}{K_H}$$

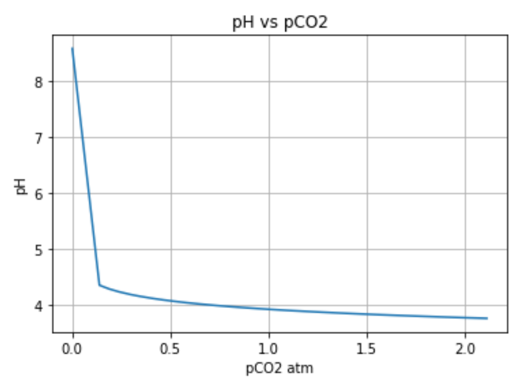
Donde *kh = 29.76 ATM/(mol/l)*

The corresponding equilibrium equations together with the ratio *[H+][OH−] = 10−14* and the neutrality condition *[H+] = [OH−] + [HCO−3] + 2 [CO2−3] result* in six equations for the six unknowns [CO2]. If we disregard the values of *[CO2−3]* we get simpler equations and end up with the following table.

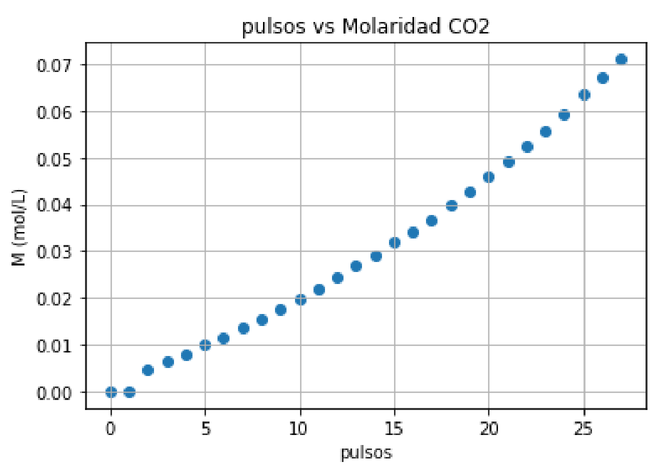
P_{CO_2} (atm)	pH	$[CO_2]$ (mol/L)	$[H_2CO_3]$ (mol/L)	$[HCO_3^-]$ (mol/L)
3.5×10^{-4}	5.65	1.18×10^{-5}	2.00×10^{-8}	2.23×10^{-6}
10^{-3}	5.42	3.36×10^{-5}	5.71×10^{-8}	3.78×10^{-6}
10^{-2}	4.92	3.36×10^{-4}	5.71×10^{-7}	1.19×10^{-5}
10^{-1}	4.42	3.36×10^{-3}	5.71×10^{-6}	3.78×10^{-5}
1	3.92	3.36×10^{-2}	5.71×10^{-5}	1.20×10^{-4}
2.5	3.72	8.40×10^{-2}	1.43×10^{-4}	1.89×10^{-4}
10	3.42	0.336	5.71×10^{-4}	3.78×10^{-4}

Since we already have the formulas, I created a program in Python to graph these components as a function of partial pressure





By combining this program with the pressure measurements discussed above, we can estimate the molarity of CO2 for each pressure point.



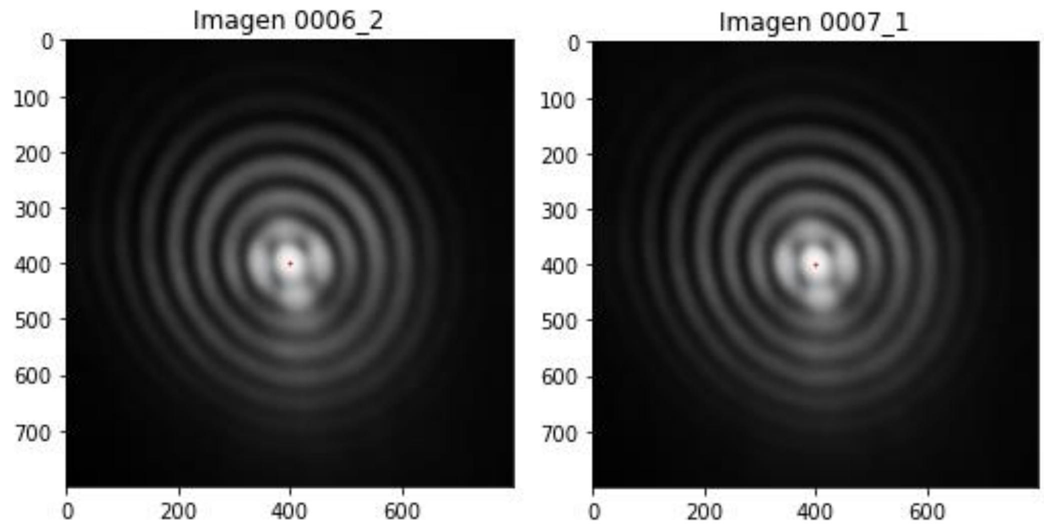
Code used: presion_teorica.py

Diffraction Patterns with White Light in Water-Methanol Mixtures

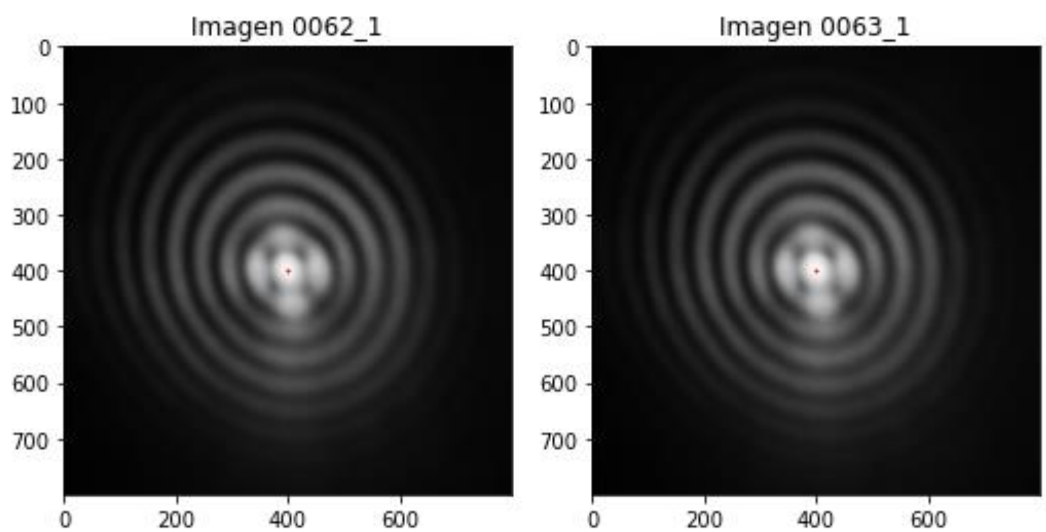
In order to obtain more information about the mixture, we performed a pattern analysis. For this analysis, the highest concentration of *CO2* in the mixture was 0.042 M and no differences between the patterns were detected.

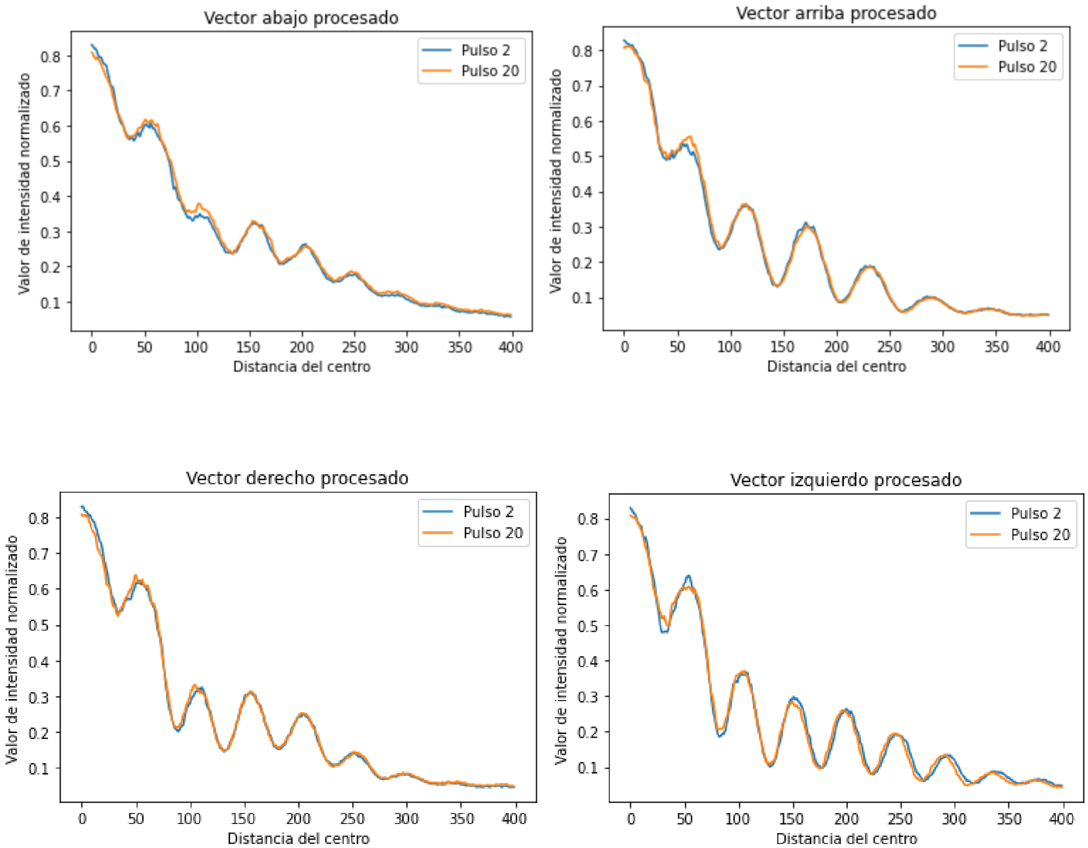
To analyze them, 2 pulse decade photos were averaged and 4 vectors from different directions were analyzed.

Pulse 2



Pulse 20

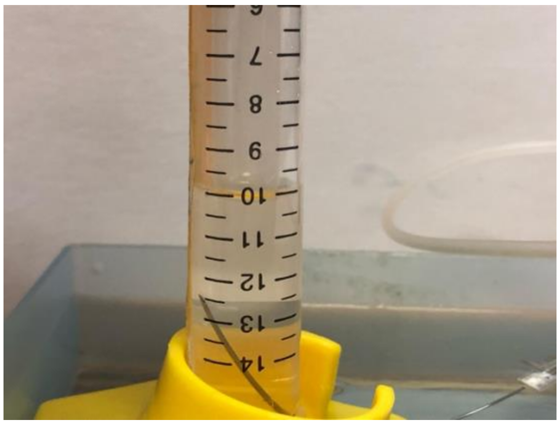


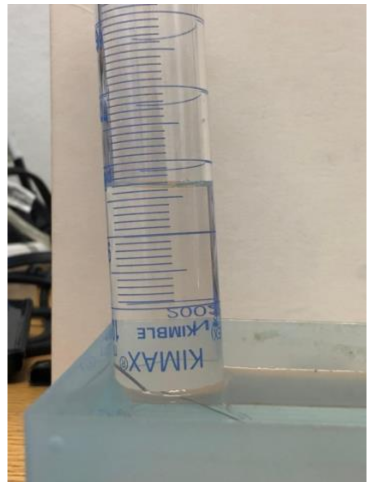


Code used: tres_pulsos_expanded.py

CARBOMED Study

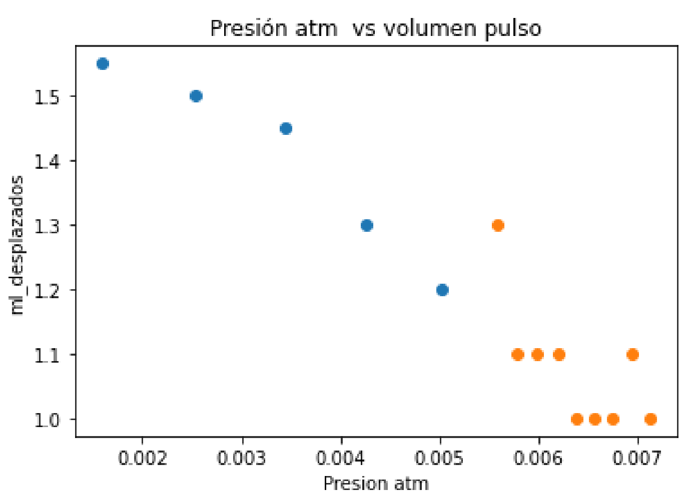
We performed the suggested experiment to observe the displaced volume and obtained the following results





We observed that the volume indicated by the CARBOMED was not coming out and not only that, when we repeated the experiment with a different specimen, we saw that the volume that came out was different.
In the large specimen, it was seen that approximately 50% of what the CARBOMED said was coming out, in the small specimen it was about 75%.

The explanation given was that the volume of CO_2 injected depended on the pressure at the tip of the syringe. This pressure was calculated through the hydraulic pressure formula. The blue dots were obtained from the small specimen and the orange dots from the large specimen.

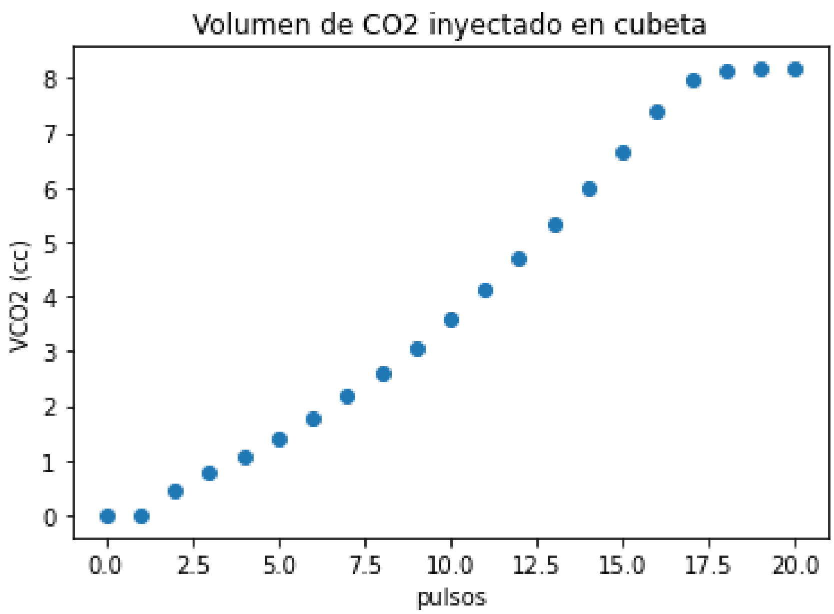


Code used: experimento_probeta.py

Future Measurements

Because the flow wasn't constant or predictable very accurately, we decided to constantly measure the pressure and calculate the volume of CO_2 injected from that.

For a measurement of interference patterns and temperature performed on the optical table, the following pressure measurements were obtained, and the volume of accumulated CO_2 as well as the volume of each pulse is shown below.

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 RESULTADOS CUBETA

Vol de CO2 inyectado en pulso 1: 0.0000 cc
Vol de CO2 inyectado en pulso 2: 0.4442 cc
Vol de CO2 inyectado en pulso 3: 0.3258 cc
Vol de CO2 inyectado en pulso 4: 0.2962 cc
Vol de CO2 inyectado en pulso 5: 0.3554 cc
Vol de CO2 inyectado en pulso 6: 0.3554 cc
Vol de CO2 inyectado en pulso 7: 0.4146 cc
Vol de CO2 inyectado en pulso 8: 0.4146 cc
Vol de CO2 inyectado en pulso 9: 0.4442 cc
Vol de CO2 inyectado en pulso 10: 0.5627 cc
Vol de CO2 inyectado en pulso 11: 0.5331 cc
Vol de CO2 inyectado en pulso 12: 0.5627 cc
Vol de CO2 inyectado en pulso 13: 0.6219 cc
Vol de CO2 inyectado en pulso 14: 0.6811 cc
Vol de CO2 inyectado en pulso 15: 0.6515 cc
Vol de CO2 inyectado en pulso 16: 0.7404 cc
Vol de CO2 inyectado en pulso 17: 0.5627 cc
Vol de CO2 inyectado en pulso 18: 0.1777 cc
Vol de CO2 inyectado en pulso 19: 0.0296 cc
Vol de CO2 inyectado en pulso 20: 0.0000 cc
```

Code used: vol_CO2_pulso.py