Temperature Dependence of Carbonation in Beer

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Introduction

Beer production happens in two processes, fermentation and carbonation. In fermentation, the yeast converts the glucose in wort to ethyl alcohol and CO_2 gas. Once the deired specific gravity, or concnetration of alcohol, is reached, the CO_2 vent is capped, and the increasing pressure creates carbonation.[1] Temperature of fermatation affects the speed of the process and the flovor of the beer. The question is, what is the effect of temprature on carbonation.

Carbonation happens when CO_2 dissovles in another liquid. This process is a function of the temperature and pressure of the system. In this paper, I will be invesitgating the temperature dependence of carbonation in beer and asking if carbonation is more effective at high or low temperatures. To answer this question, I model carbonation as a function of temperature using Henry's Law and the Van't Hoff equationand compare it to solubility data for both CO_2 in water and CO_2in a solution of water and ethonol.

Model

Henry's Law, a common model for solubility of gas in liquid, states that concentration of the gas is directly proportional to it's partial pressure above the liquid.[2] This law only holds true for dilute solutions and low gas pressures.[3]

This relationship can be stated as $C = H \bullet P_{gas}$, where C is the solubility of thee gas at a fixed temperature in a particular solvent (in M or mL of gas/L), H Henry's law constant, and P_{gas} is the partial pressure of gas (often in atm).[4]

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[1] "How Beer Works," *How Stuff Works*. 2020. https://science.howstuffworks.com/innovation/edible-innovations/beer4.htm

[2] "Henry's Law," *Chemistry LibreTexts.* URL.

[3] "Henry's Law," *Encyclopedia Britannica*. https://www.britannica.com/science/Henrys-law

[4] "Henry's Law," *Chemistry LibreTexts.* URL.

$H$is a function of temperature, the relationship is one of exponential decay and is described by the Van't Hoff equation (shown in **Figure 1**) where H° is Henry's constant at reference temperature T°, $\Delta_{sol}H$ is the enthalpy of dissolution, which is found based on the material identity of the solute, not the solvent.[5]

$$H(T) = H^{\circ} \exp\left[\frac{-\Delta_{\text{sol}}H}{R}\left(\frac{1}{T} - \frac{1}{T^{\circ}}\right)\right].$$

Figure 1 Van't Hoff equation for temprature dependence of Henry's constant.[6]

The reference value for $H \circ$ at $T^{\circ} = 298.15\ K$ for CO_2 is $H^{\circ} = 3.4\times10^{-2}\ \frac{mol}{L\bullet atm}$.[7] The value of $-\frac{\Delta_{sol}H}{R}$for CO_2 is $2400\ K$.[8] With these values filled in, I substituted this function of temperature for Henry's constant, H, in Henry's Law, and since the values I will validate this model against are measured at $1\ atm$, P_{gas} will be $1\ atm$.

Thus the final equation for temperature dependent solubility is

$$C = H(T) = 3.4\times10^{-2}\ \frac{mol}{L\bullet atm} \bullet exp\left(\frac{-\Delta_{sol}H}{R}\left(\frac{1}{T} - \frac{1}{298.15\ K}\right)\right)$$

When plotted, shown in **Figure 2**, we find that the relationship is that of an exponential decay function.

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[5] Smith, Francis, and Allan Harvey. "Avoid Common Pitfalls When Using Henry's Law." URL

[6] "Henry's Law," *Wikipedia*. URL.

[7] Sander, R. "Compilation of Henry's law constants (version 4.0) for water as solvent," *Atmos. Chem. Phys.*, 15 (8): 4399–4981, (2015). URL.

[8] "Henry's Law," *Wikipedia*. URL.

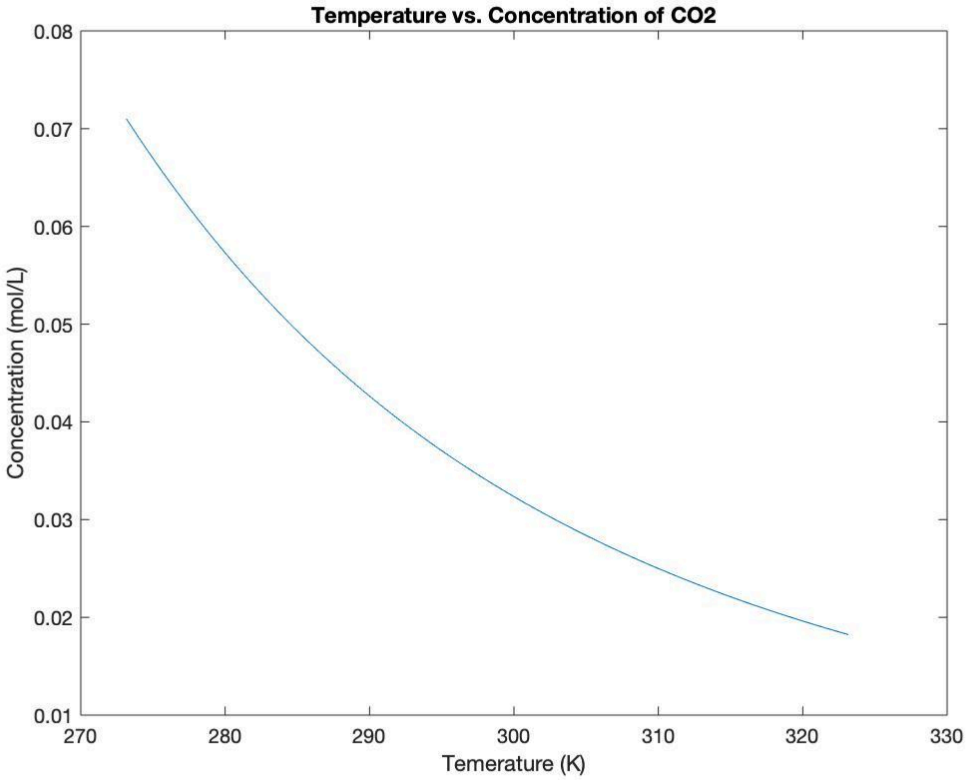

Figure 2 plot of carbonation as a function of temperature using Van't Hoff equation and Henry's Law.

Validation

To validate this model, I compared it to datasets comparing temperature to CO_2 concentration in water and in a solution of $27.40\ (v/v)$ethanol to water.[9]

The concentration values are expressed as the Bunsen coefficient. The Bunsen coefficinet describes solubility (v/v) in reference to a specified temperatue, usually STP $(273.15\ K)$,[10] and a specified pressure, in this case, $1\ atm$.[11] The conversion of the Bunsen coefficient to Henry's law constant is as follows in **Figure 3** where $R\ =\ 0.8206\frac{L\bullet atm}{mol\bullet K}$.

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[9] Speers, R. "Carbon Dioxide Solubility in Beer," *Journal of the American Society of Brewing Chemists* (2013).

[10] "Henry's Law," *Wikipedia*. URL.

[11] Speers, R. "Carbon Dioxide Solubility in Beer," *Journal of the American Society of Brewing Chemists* (2013).

$$H^{cp} = \alpha \frac{1}{RT^{\mathrm{STP}}}$$

Figure 3 conversion of Bunsen coefficient, α, to Henry's law constant H^{cp}in units of $\frac{mol}{L \bullet atm}$.[12]

Based on this conversion, **Figure 4** shows the comparison of data with water as a solvent to the mathematical model found above.

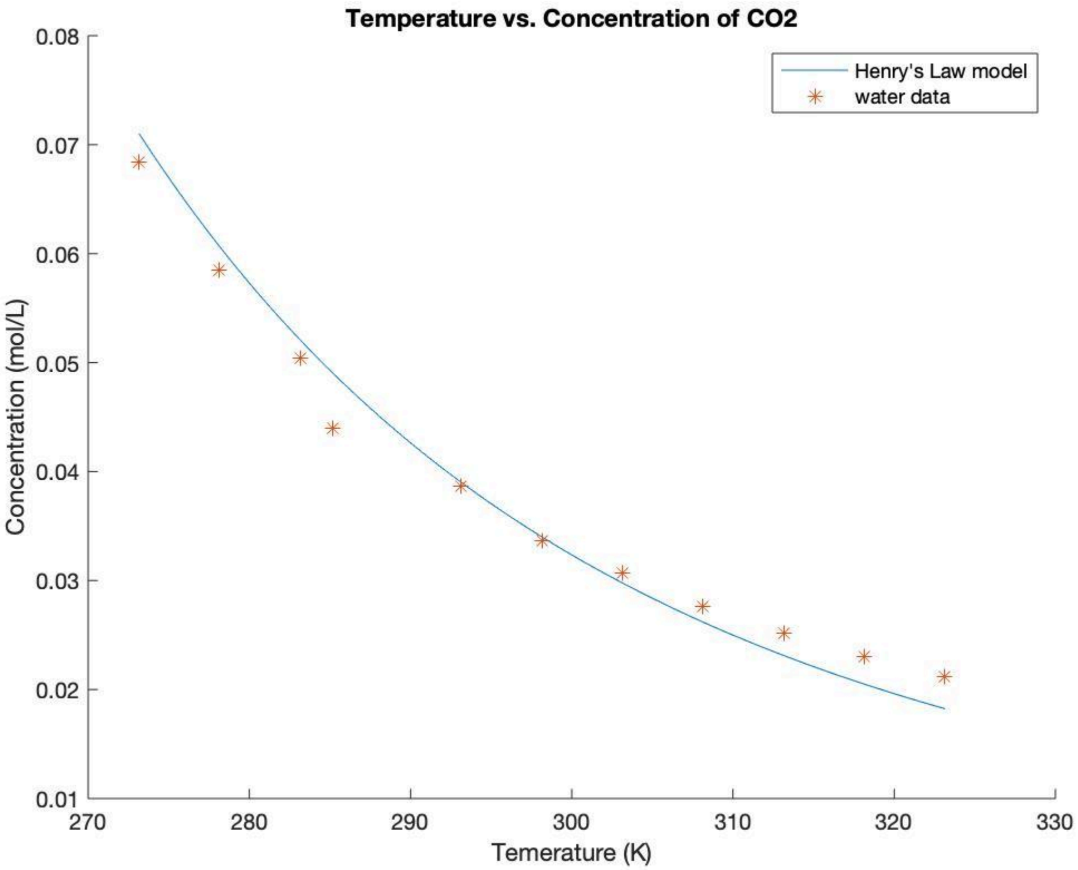

Figure 4 model plotted against concentration data for water as a solvent

Similarly, **Figure 5** shows converted concentration values versus temperature of CO_2in a solution of $27.04\ (v/v)$ ethanol.

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[12] “Henry’s Law,” *Wikipedia*. URL.

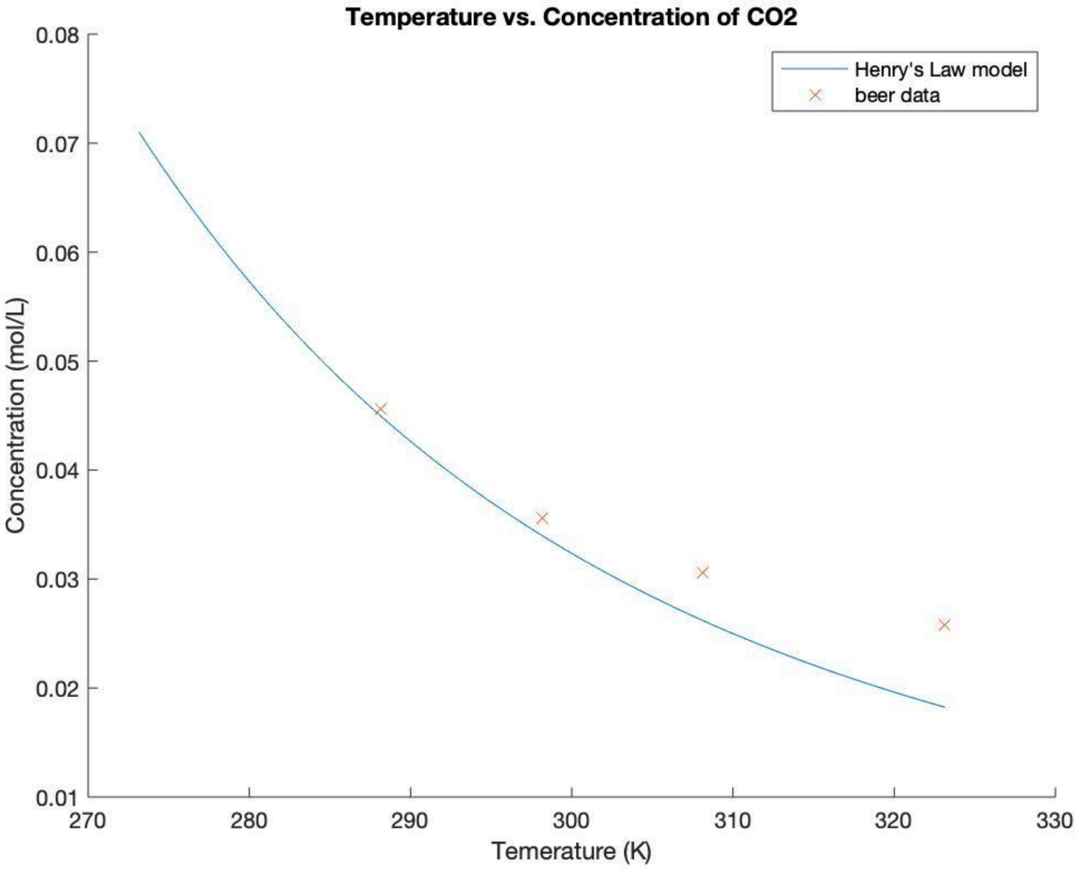

Figure 5 model plotted against concentration data for solution of $27.04\ (v/v)$ as a solvent.

Figure 6 shows both of these datasets overlaid with the Van't Hoff and Henry's law model of carbonation.

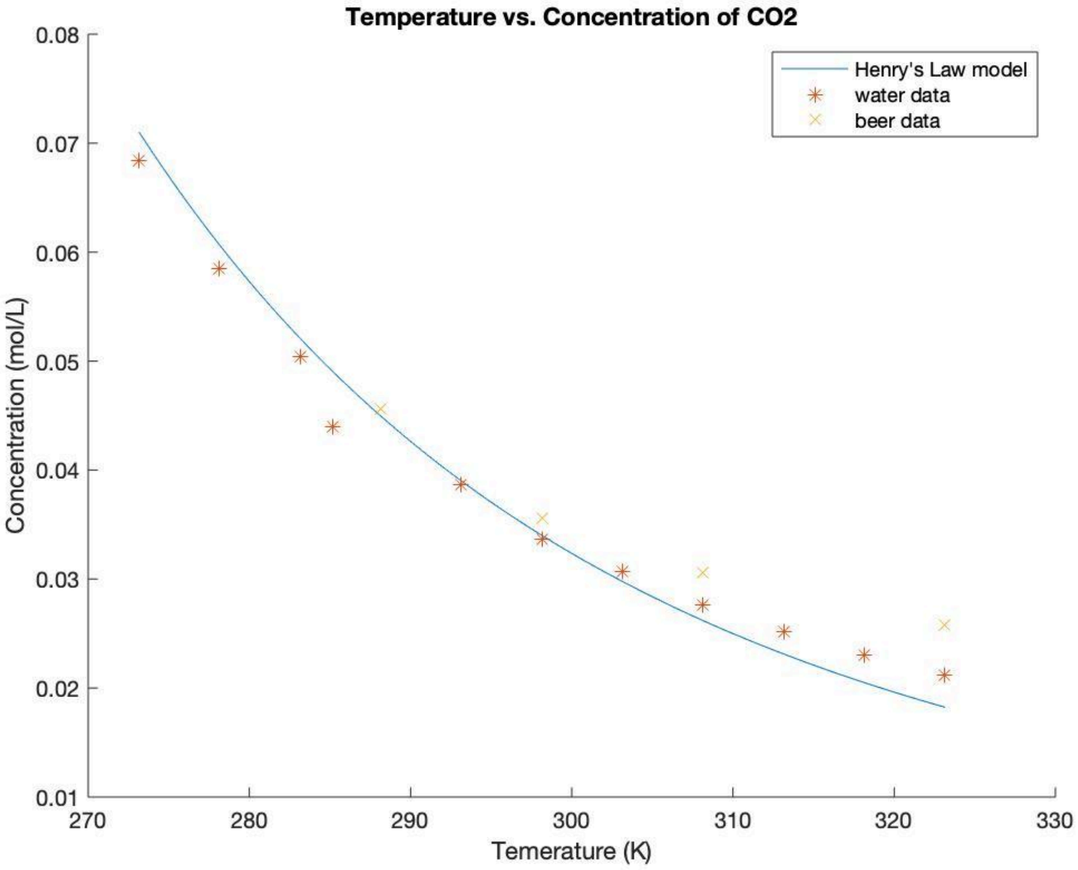

Figure 6 model plotted against concentration data for water and solution of $27.04\ (v/v)$as solvents.

Discussion

Looking at **Figure 4**, on inspection, the model fairly is accurate for water as a solvent, but the slope of the model is steeper than that of the data starting at $300\ K$. This is likely becasue of a slight change due to temperature of the enthalpy of dissolution, which the Van't Hoff equation depends on. Although the enthalpy of dissolution is reletively constant as temperature changes,[13] it is dependent on internal energy which will be affected by larger changes in temperature.[14] Mathematically explained, since the slope becomes less extreme, the numberater of the exponent must increase. The only value that could change to account for this is the enthalpy of dissolution, suggesting that the enthalpy of dissolution increases with temperature.

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[13] "Henry's Law," *Wikipedia*. URL.

[14] "Enthalpy," *Encyclopedia Britannica*. URL.

Figure 5 shows that the ethanol solution shows a similar trend of deviating from the model with a less extreme slope, also deviating at around $300\ K$. Since this type of deviation is consistent acrosss solvents and consistently deviates at around $300\ K$ for both solvents, it is most likely to be accounted for by a change in enthalpy of dissolution, a property that depends on material identity.

Looking at **Figure 6,** the carbonation in ethanol solution has an even less extreme slope than the carbonation in water, enthalpy of dissolution begins to change based on material identity of the solvent, not just the solute, at around $300\ K$.

Although the results reveal inaccuracy in the Van't Hoff equation and Henry's law model at higher temperatures, the concentration of $CO_2$is highest at lower temeratures, suggesing that carbonation is most effective at lower temperatures.

The inaccruacy at higher temperatures will have little effect on the model unless the targeted temperatues are over $300\ K$ or $27\ \circ C$. The typical beer fermentation temperature is around $20 - 22\ \circ C$[15], just on the cusp of when this model becomes inaccurate. At that temperature, a good model would also account for the change in temperature and the material identity of the solvent when calculating the enthalpy of dissolution.

Appendix: Simulation Code

```
% -----------------Model---------------

% define system parameters
delHR = 2400;  % (K)
H_o = 3.4e-2;  % (mol/L*atm)
T_o = 298.15;  % (K)
P = 1;         % pressure (atm)

% temprature span for plotting
T_span = [273.15:.5:323.15];

% concentaration (mol/L) as a function of temprature (K)
c_model = H_o*P*exp(delHR*P*(1./T_span - 1/T_o))

% -----------------Validation---------------
T_data_c = [0, 5, 10, 12, 20, 25, 30, 35, 40, 45, 50]; % temp data (degrees C)
T_data = T_data_c + 273.15; % convert to K

bunsen_data = [1.534, 1.310, 1.131, .985, .866, .755, .687, .620, .564, .516, .476];

% convert to conentration
R = 0.082057366080960;     % L*atm/mol*K
T_stp = 273.15;            % K
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[15] "Controlling Fermentation Temperature," *Brew Your Own*. URL.

```
H_cp_data = bunsen_data.*(1/(R*T_stp));
c_data = H_cp_data*P

% beer data
T_beer_c = [15, 25, 35, 50];
T_beer = 273.15 + T_beer_c


bunsen_beer = [1.022, .798, .685, .578];
H_cp_beer = bunsen_beer.*(1/(R*T_stp));

c_beer = H_cp_beer*P;


% -----------------Plotting---------------

figure
plot(T_span, c_model)
xlabel("Temerature (K)")
ylabel("Concentration (mol/L)")
title("Temperature vs. Concentration of CO2")

figure
hold on
plot(T_span, c_model)
plot(T_data, c_data, "*")
legend("Henry's Law model", "water data")
xlabel("Temerature (K)")
ylabel("Concentration (mol/L)")
title("Temperature vs. Concentration of CO2")

figure
hold on
plot(T_span, c_model)
plot(T_beer, c_beer, "x")
legend("Henry's Law model", "beer data")
xlabel("Temerature (K)")
ylabel("Concentration (mol/L)")
title("Temperature vs. Concentration of CO2")

figure
hold on
plot(T_span, c_model)
plot(T_data, c_data, "*")
plot(T_beer, c_beer, "x")
legend("Henry's Law model", "water data", "beer data")
xlabel("Temerature (K)")
ylabel("Concentration (mol/L)")
title("Temperature vs. Concentration of CO2")
```