CO_2 solubility: The epic battle between ions and CO_2 for water and energy

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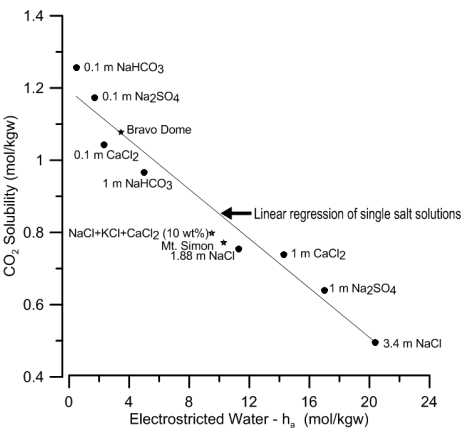
We propose a novel approach to predict CO_2 solubility using the concentration of electrostricted water per kg of water, (h_a) based on the hydration number of the dissolved electrolytes. We evaluated the energy (ΔG_{hydr}) required to remove water from hydrated ions to form the characteristic water cage around CO_2. The resulting model can be used to predict CO_2 solubility in both single salt and complex solutions.

We measured CO_2 solubility in water and NaCl, $CaCl_2$, Na_2SO_4 and $NaHCO_3$ solutions and correlated CO_2 solubility to h_a ($R^2 = 0.96$) at 60°C and 6.7MPa CO_2 fugacity (f). CO_2 solubility is also correlated to ΔG_{hydr} ($R^2 = 0.91$).



We evaluated over 500 CO_2 solubility data points from literature combined with our own experimentally-determined data and used moderated multiple regression to generate a predictive CO_2 solubility model with only 4 variables: h_a, ΔG_{hydr}, *f*, and T. The resulting model uses literature available parameters, making it easily extensible with added electrolytes, unlike other typical solubility models such as the Pitzer model. In predicting CO_2 solubility in 3 mixed brines our model produced equalivalent or lower errors than the Pitzer equation.