

## Converting eosGP CO<sub>2</sub> readings to dissolved CO<sub>2</sub> concentrations

### Introduction

The Eosense eosGP CO<sub>2</sub> concentration probe measures CO<sub>2</sub> concentration in the soil, and to a maximum depth of 3 meters in water. Measurements of CO<sub>2</sub> in the water column require corrections to account for the combined atmospheric and water pressure (hydrostatic pressure). Similarly, to calculate dissolved gas concentrations in mg/L or similar non-relative concentrations, researchers must account for additional water parameters. This application note demonstrates how to apply these corrections to eosGP measurements collected in aqueous environments.

### Pressure Dependence of CO<sub>2</sub> Measurements

Non-dispersive infrared sensors like the eosGP measure gas density in the sensor head and are therefore affected by ideal gas law parameters, namely pressure and temperature. Eosense's calibration includes a correction for temperature but pressure corrections are left to the user because there is no on-board pressure reading available. When using the eosGP in air or soil, the concentrations must be corrected by using the pressure at the time of measurement and the calibration pressure.

$$\text{CO2}_{\text{corrected}} = \text{CO2}_{\text{measured}} \frac{P_{\text{ref}}}{P_{\text{measured}}}$$

For example, an eosGP calibrated in Halifax, Nova Scotia (~101 kPa) measuring atmospheric concentrations of CO<sub>2</sub> in Boulder, Colorado (~400 ppm CO<sub>2</sub>, ~84 kPa) would read approximately 332 ppm CO<sub>2</sub> due to the difference in air pressure. To correct we would apply the equation above:

$$\text{CO2}_{\text{corrected}} = 332 \text{ ppm} \frac{101.3 \text{ kPa}}{84 \text{ kPa}} = 400 \text{ ppm}$$

Similarly, when measuring CO<sub>2</sub> concentrations in the water column the user needs to correct for the hydrostatic pressure.



### Accounting for Water Pressure

To determine the true CO<sub>2</sub> concentration in the water column, the user must account for the hydrostatic pressure. Hydrostatic pressure is defined as:

$$P = \rho g h$$

where  $\rho$  is the density of water,  $g$  is the gravitational acceleration and  $h$  is the height of the water column. For example, the pressure 1 meter below the surface of 4°C distilled water is:

$$P = 1000 \text{ kg/m}^3 \times 9.8 \text{ m/s}^2 \times 1 \text{ m} = 9800 \text{ Pa}$$

Although hydrostatic pressure will vary with temperature and water composition, in most cases it is only a few percent. As a practical example, if an eosGP at a water depth of 1.5 meters reads a value of 1500 ppm CO<sub>2</sub>, the true concentration is 1310 ppm, as per the calculation below.

$$P = 1000 \text{ kg/m}^3 \times 9.8 \text{ m/s}^2 \times 1.5 \text{ m} = 14700 \text{ Pa}$$

$$\text{CO2}_{\text{corrected}} = 1500 \text{ ppm} \frac{101.3 \text{ kPa}}{101.3+14.7 \text{ kPa}} = 1310 \text{ ppm}$$

## Conversion to pCO<sub>2</sub> and Aqueous Concentration

Converting CO<sub>2</sub> concentration (ppm) measurements in the water column to the partial pressure of CO<sub>2</sub> is done by considering the summed atmospheric and hydrostatic pressures:

$$p\text{CO}_2 = \text{CO}_2 (P_{\text{atmospheric}} + P_{\text{hydrostatic}}) \times 10^{-6}$$

where pCO<sub>2</sub> is given in kPa (or the units in which the pressures were prescribed, eg. atm). Converting to dissolved CO<sub>2</sub> concentration is less straightforward and requires knowledge of the water temperature, and the associated Henry's law coefficients. To calculate the molarity of CO<sub>2</sub> dissolved in water (mols of solute per litre of solution), we use:

$$\text{CO}_2 \text{ (M)} = p\text{CO}_2 / K_H$$

where K<sub>H</sub> is the Henry's law coefficient for CO<sub>2</sub>-H<sub>2</sub>O equilibrium at a given temperature (L atm mol<sup>-1</sup>). Henry's law coefficients are commonly calculated using thermodynamic laws with empirically derived rate coefficients. The following references are useful for determining the correct K<sub>H</sub> values at various water temperatures:

Plummer, L.N., Bundenberg, E. (1982) The solubilities of calcite, aragonite and vaterite in CO<sub>2</sub>-H<sub>2</sub>O solutions between 0 and 90C, and an evaluation of the aqueous model for the system CaCO<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O. *Geochimica et Cosmochimica Acta*, 46, 1011-1040.

Sander, R. (1999) *Compilation of Henry's Law Constants for Inorganic and Organic Species of Potential Importance in Environmental Chemistry*, Retrieved Feb 19, 2018 from <http://www.henrys-law.org/henry-3.0.pdf>.

The approximate K<sub>H</sub> coefficients for CO<sub>2</sub>-H<sub>2</sub>O equilibrium at several water temperatures are shown in the table to the right. These calculations were made using the Van't Hoff equation:

$$K_H(T) = K_H^* \exp\left(k_T \left(\frac{1}{T} - \frac{1}{T^*}\right)\right)$$

Where K<sub>H</sub>(T) is the Henry's law coefficient as a function of temperature, K<sub>H</sub><sup>\*</sup> is the coefficient at T<sup>\*</sup>=298.15 K (K<sub>H</sub><sup>\*</sup>=29) and k<sub>T</sub> is the rate constant (2400 for CO<sub>2</sub>).

Temperature (°C)	K <sub>H</sub> (L atm mol <sup>-1</sup> )
0	60.6
5	51.7
10	44.4
15	38.3
20	33.3
25	29.0
30	25.4
35	22.3
40	19.7

Many researchers will report in g/L or mg/L rather than mol/L, the conversion from molality is simple and only requires multiplying by the molar mass of the solute (44.01 g/mol)

$$\text{CO}_2 \text{ (g/L)} = \text{CO}_2 \text{ (M)} \times 44.01 \text{ (g/mol)}$$

## Conclusion

The eosGP measures CO<sub>2</sub> concentrations in soil and to a depth of 3 meters in water. In the latter case, researchers must correct for both atmospheric and hydrostatic pressures to produce accurate measurements. Depending on the desired units, further corrections may need to be applied based on Henry's law and molecular mass.