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Vaisala CARBOCAP® Carbon Dioxide Sensors:

What is CO_2?

This document describes the properties of carbon dioxide (CO_2) and presents ideal gas law, unit conversion and gas dilution theory to support gas sampling issues in CO_2 measurements.

What is CO_2?

Carbon dioxide (CO_2) is a colorless gas consisting of one carbon and two oxygen atoms. CO_2 exists in gas state above -78.5°C and in solid state (dry ice) below -78.5°C. CO_2 changes from solid to gas by sublimation.

In nature, plants use CO_2 in photosynthesis, where CO_2 and water are combined using sun light as energy to produce sugars (and oxygen). The reaction can be written in a general form:

$$6\ CO_2 + 6\ H_2O \underset{respiration}{\overset{photosynthesis}{\rightleftarrows}} C_6H_{12}O_6 + 6\ O_2$$

In fact, CO_2 is introduced in the greenhouse air to maintain plant growth, since plants grow up to 50% faster in elevated CO_2 concentrations. The opposite reaction to photosynthesis, respiration, takes place in all living organisms.

In addition to its vital role in photosynthesis, respiration and carbon cycle, CO_2 has many industrial applications. Solid and liquid CO_2 are used in refrigeration and cooling. In beverage industry, CO_2 gives the fizz to the drinks and prevents bacterial and fungal growth in soft drinks, beer and wine. CO_2 is an environmentally friendly propellant in aerosols and due to its unreactive nature it is used as an inert gas in various processes, packaging and fire extinguishers, to mention some applications. CO_2 is produced in combustion processes of carbon containing material.

Effects of CO_2

Typical atmospheric CO_2 concentration is 350-450 ppm. CO_2 is a non-toxic and non-flammable gas. However, it doesn't support life and exposure to elevated CO_2 concentrations can induce a risk to life. The effects of CO_2 concentrations on people are summarized in Table 1.

Table 1. Effect of CO_2 concentrations on people.

Concentration	Effect
350-450 ppm	Typical atmospheric
600-800 ppm	Acceptable indoor air quality
1000 ppm	Tolerable indoor air quality
5000 ppm	Average exposure limit over 8 hours
600-30 000 ppm	Concern, short exposure only
3-8%	Increased respiration and headache
above 10%	Nausea, vomiting, unconsciousness
above 20%	Rapid unconsciousness, death

To ensure the safety of the people in facilities having a potential risk for CO_2 leakage, CO_2 transmitters should be installed as close to the potential leakage points as possible. CO_2 is heavier than air, therefore it sinks and pools low to the ground, displacing the oxygen. The CO_2 transmitter installations should always be based on risk assessment.

Physical properties of CO_2

CO_2 absorbs light in the infrared (IR) region, see Figure 1. This absorption can be utilized to measure volumetric concentration of CO_2. Vaisala CARBOCAP® is utilizing this absorption in the silicon-based non-dispersive infrared CO_2 sensors.

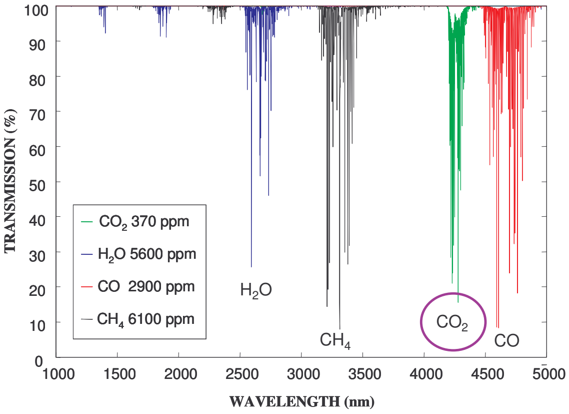

Figure 1. IR absorption of some gases.

This IR absorption of CO_2 is partly responsible for the greenhouse effect. The greenhouse effect is a property of any planetary atmosphere, which results in the temperature of the planet surface being higher than without the atmosphere. Any gas absorbing sun light causes greenhouse effect, the most important greenhouse gases on planet earth being water vapor, CO_2 and methane, all absorbing in the IR region.

Some physical properties of CO_2 are collected to Table 2.

Table 2. Physical properties of CO_2.

CO_2 Physical Properties	
Molecular weight	44.01 g/mol
Gas density (1013 bar, 15℃)	1.87 kg/m^3
Solid density	1562 kg/m^3
Specific gravity (air = 1) (1.013 bar, 21 ℃)	1.521
Volume of 1 kg of dry ice in gas phase	0.518 m^3
Critical temperature and pressure	31℃, 73.825 bar
Triple point temperature and pressure	-56.6℃, 5.185 bar
Sublimation point	-78.5℃

Ideal gas law

Ideal gas law is an equation describing the state of a hypothetical ideal gas. The ideal gas law relates the state of a certain amount of gas to its pressure, volume, and temperature according to the equation:

$$pV = nRT$$

where
p = pressure [Pa]
V = volume of the gas [m^3]
n = amount of gas [mol]
R = universal gas constant (= 8.3145 J/mol K)
T = temperature [K]

Ideal gas is a hypothetical gas having zero volume identical particles with no intermolecular forces. The ideal gas atoms or molecules are assumed to undergo elastic collisions with the container walls. In reality, gases do not behave exactly like ideal gases, but this approximation is often good enough to describe real gases.

Most gas sensors give out a signal proportional to the molecular density (molecules/cm^3), even though the reading is expressed in *ppm* units. Changing p and/or T changes the molecular density of the gas according to the ideal gas law. This is seen in the sensor *ppm* reading. In exact terms this is an error in the measurement, since the concentration of the gas (in *ppm* units) doesn't change with varying temperature and pressure.

The ideal gas law can be used to calculate the (molecular) density of a gas at given t and p, when the density at Standard Ambient Temperature and Pressure (SATP) conditions is known. Replacing n by ($\rho V/M$) and assuming molar mass M constant in the two different conditions the equation can be written as:

$$\rho(t,p) = \rho(25°C, 1013hPa) \times \frac{p}{1013} \times \frac{298}{(273+t)}$$

where
ρ = gas volume concentration [ppm or %]
p = ambient pressure [hPa]
t = ambient temperature [°C]

This density formula can be used to calculate how the gas sensor reading changes as a function of t and p. The data can also be used to correct the gas sensor reading for t and p variations.

Table 3 shows how the reading of a 1 000 ppm (at SATP) concentration changes with t and p according to ideal gas law.

Table 3. Reading of a 1 000 ppm concentration (SATP) in different temperature and pressure conditions.

		Temperature (℃)									
		-20	-10	0	10	20	25	30	40	50	60
Pressure (hPa)	700	814	783	754	728	703	691	680	658	638	618
	800	930	895	862	832	803	790	777	752	729	707
	900	1046	1007	970	936	904	888	874	846	820	795
	1000	1163	1119	1078	1039	1004	987	971	940	911	883
	1013	1178	1133	1092	1053	1017	1000	983	952	923	895
	1100	1279	1230	1185	1143	1104	1086	1068	1034	1002	972
	1200	1395	1342	1293	1247	1205	1185	1165	1128	1093	1060
	1300	1512	1454	1401	1351	1305	1283	1262	1222	1184	1148

Unit conversions

CO_2 concentration in the air is 350-450 ppm. The ppm unit is an abbreviation from parts per million, thus 1 ppm means one part in 1×10^6. Thus 1% = 10 000 ppm.

The following tables can be used to convert pressure, temperature, flow rate and length units from SI units to other units and vice versa. To make a unit conversion in pressure, length and flow rate, select the known unit from the left column and multiply by the number in the corresponding cell for unit conversion. For temperature conversions, the formulas are given in Table 4.

Table 4. Unit conversion tables for pressure, temperature, length and flow rate.

Pressure

From \ To	bar	psi	torr	kPa	atm
bar	1	14.5	750	100	0.987
psi	0.0690	1	51.7	689	0.0680
torr	0.00133	0.0193	1	0.1330	0.00132
kPa	0.0100	0.0015	7.5188	1	0.00987

Temperature

K (Kelvin)	℃ + 273.15
F (Fahrenheit)	(℃ + 17.78) × 1.8
C (Celsius)	0.56 × ℉ - 17.78

Flow rate

From \ To	l/min	scfh	scfm
l/min	1	2.2	0.0353
scfh	0.472	1	0.0167
scfm	28.3	60	1

Length

From \ To	m	ft	in
m	1	3.28	39.4
ft	0.305	1	12
in	0.0254	0.0833	1

Drying a wet gas sample

Processing the ideal gas law a bit further provides a way to understand what happens when the composition of a gas mixture is varied in constant *p, T* and *V*. All the molecules in a gas mixture occupy the same system volume (*V* is the same for all gases) and they exist in the same *T*. The ideal gas law can be modified to:

$$p = (n_{gas1} + n_{gas2} + n_{gas3} + \ldots n_{gasn}) \times \frac{RT}{V}$$

$$p = p_{gas1} + p_{gas2} + p_{gas3} + \ldots p_{gasn}$$

The lower equation is called Dalton's Law of Partial Pressure. It states that the pressure of a gas mixture is the sum of the partial pressures of the components in the mixture.

This information is useful when taking account the influence of water vapor on CO_2 sensor reading. For example, if water vapor is added to a dry gas in constant *p*, *T* and *V*, water replaces some of the other gas molecules in the mixture.

The dilution effect of water can be estimated using Table 5, which contains the dilution coefficients for gas concentrations when drying a gas sample. Dewpoint (Td, at 1013 hPa) or the H_2O concentration of the wet sample is chosen from the horizontal axis and the dewpoint or H_2O concentration of the dried sample on vertical axis.

Table 5. Dilution coefficients for drying a wet gas sample.

	Td(℃)	-40	-30	-20	-10	0	10	20	30	40	50	60
Td(℃)	ppm H_2O	127	377	1020	2580	6060	12200	23200	42000	73000	122000	197000
-60	11	0.9999	0.9996	0.999	0.997	0.994	0.988	0.977	0.958	0.927	0.878	0.803
-50	39	0.9999	0.9997	0.999	0.997	0.994	0.988	0.977	0.958	0.927	0.878	0.803
-40	127	1.0000	0.9997	0.999	0.998	0.994	0.988	0.977	0.958	0.927	0.878	0.803
-30	377		1.0000	0.999	0.998	0.994	0.988	0.977	0.958	0.927	0.878	0.803
-20	1020			1.000	0.998	0.995	0.989	0.978	0.959	0.928	0.879	0.804
-10	2580				1.000	0.997	0.990	0.979	0.961	0.930	0.880	0.805
0	6060					1.000	0.994	0.983	0.964	0.933	0.884	0.809
10	12200						1.000	0.989	0.970	0.939	0.890	0.815
20	23200							1.000	0.981	0.950	0.901	0.826
30	42000								1.000	0.969	0.920	0.845
40	73000									1.000	0.951	0.876
50	122000										1.000	0.925
60	197000											1.000

Here is an example how to use Table 5: A gas sample is drawn from 40°C(Td) to 20°C(Td) environment. The measured gas concentration of 5.263% at 20°C(Td) means 5.00% in the 40°C(Td) environment (5.263% × 0.950 = 5.00%). This lower reading is caused by the dilution due to higher water content in 40°C(Td).