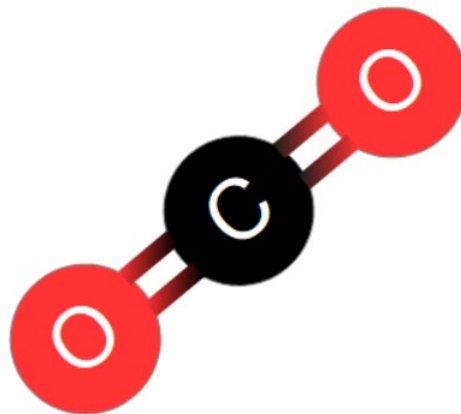# AN001: PRESSURE COMPENSATING OF A CO_2 SENSOR

ABSTRACT

Non-dispersive infra-red (NDIR) sensors work by measuring the amount of IR light absorbed by the target gas in a fixed volume. Gas concentration is proportional to the amount of light absorbed as it passes through the gas.

The amount of light absorbed by the target gas, and hence measurement accuracy, is influenced by external environmental factors. The absorption of IR light is dependent on the number of gas molecules present in the fixed volume. Three factors influence the number of molecules in this fixed space, the gas concentration, gas temperature and gas pressure. To accurately measure gas concentration, it is therefore important to understand the effects of temperature and pressure.

The general behaviour of a gas, due to changes in temperature and pressure is based on well understood laws. However, the effects of temperature and pressure on the absorption of infra-red light by gas molecules and how they influence measurement accuracy are less well understood.

This application note describes the physical effects on the gas molecules due to changes in temperature and pressure. Changes in ambient temperature and pressure will induce CO_2 concentration measurement errors unless corrected.

It also explains how CO_2 sensor measurements are affected by temperature and pressure and how these effects can be compensated for to reduce their impact on sensor accuracy.

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BASIC PRINCIPLES

All NDIR sensors measure the concentration of CO_2 in a fixed volume, which in turn is based on the number of molecules present. The more molecules there are in the fixed volume, the more IR radiation is absorbed. Both temperature and pressure influence the number of molecules present in the fixed volume and therefore, measurement accuracy will be affected unless steps are taken to compensate for these effects.

ENVIRONMENTAL FACTORS

The two environmental factors that decide the number of molecules present in a defined volume for any gas are temperature and pressure. This is defined by the ideal gas law, which combines the work of Boyle, Charles & Gay-Lussac (from the 17th, 18th & 19th centuries).

The basic principles are simple to understand; as the gas temperature increases, the molecules vibrate more and in doing so, they take up more room, and the number present in a vented fixed volume is reduced. Similarly, if the pressure is increased more molecules are pressed together and give rise to a higher number in the same volume.

GAS VIBRATIONS

Before the additional effects of temperature and pressure are analysed, it is important to review why some CO_2 molecules absorb IR radiation and some do not.

CO_2 molecules have 4 degrees of vibrational freedom. The potential gas vibrations are defined as symmetrical, asymmetrical and two types of bending. The symmetric vibrations are due to the two oxygen atoms vibrating around the carbon atom while always being an equal distance from the carbon atom. Asymmetrical vibrations are due to the carbon atom moving back and forward between the 2 oxygen atoms. The two bending vibrations, so-called degenerate bends are less distinct, but effectively either vibrate up and down or backwards and forward.

Symmetric stretch   **Asymmetric stretch**

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Figure 1: CO_2 Vibration Modes

The symmetric stretch does not create a dipole and consequently is not able to absorb any photons. It therefore does not absorb infra-red radiation. The other three vibration modes produce a dipole and absorb photons although at different frequencies. The asymmetric stretch absorbs radiation at 4.26μm, whereas the bending modes absorb at 15μm.

Most NDIR based sensors measure the absorption of photons at 4.26um, and this is due to the asymmetric stretch vibration mode. The proportion of molecules vibrating in each mode remains the same as temperature and pressure are changed.

A typical GSS sensor will contain approximately $1x10^{16}$ CO_2 gas molecules at 25°C and 1013mbar (1 atmosphere pressure) at 400ppm concentration levels.

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ABSORPTION

Absorption at 4.26µm due to the symmetric vibration mode is negligible. This is because the average position of the gas molecule is the same as symmetric bending mode case, with no dipole and hence little absorption. However, as the atoms vibrate asymmetrically and form different dipole strengths depending on the energy levels of the electrons, the gas molecules begin to absorb infra-red radiation.

The different energy levels of the molecules cause absorption at a series of distinct wavelengths as shown below in Figure 2. The effects of changes to the absorption due to pressure and increased temperature scan be seen more clearly by focusing on one specific wavelength.
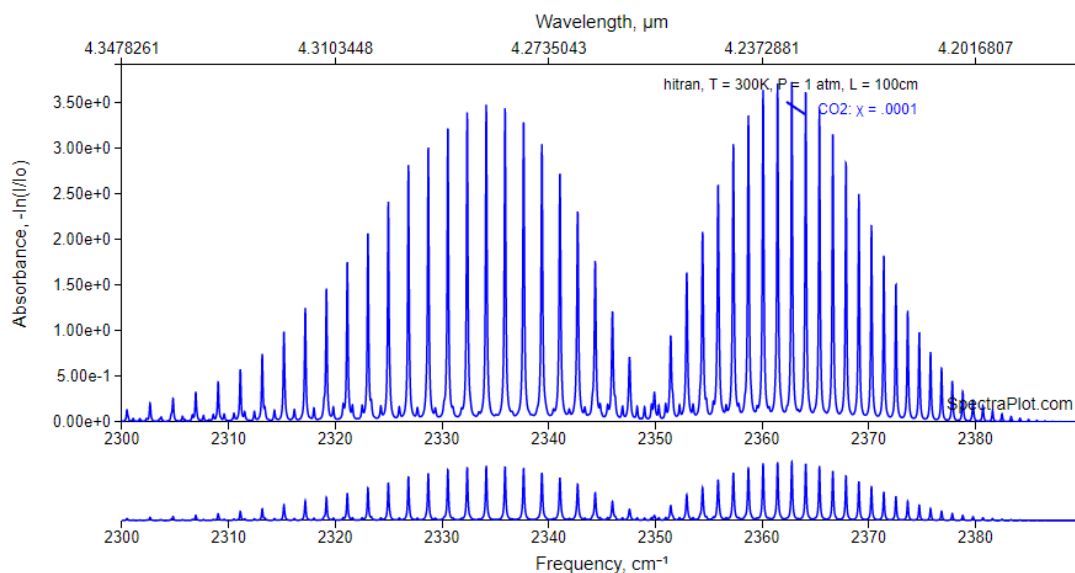

Figure 2: CO$_2$ Absorption Around 4.3µm

Figure 3 shows the impact of changes of pressure on absorption at 4.28µm. Figure 3 also shows how the absorption is affected by changing the gas pressure from 1.0 to 1.5 atmospheres, with all other parameters unchanged. Although the peak absorption does not change significantly, the width of the peak increases as the pressure increases. This is caused by the increased collisions as the molecules vibrate, causing electron energy levels to vary and the gas absorbing photons over a slightly greater bandwidth.

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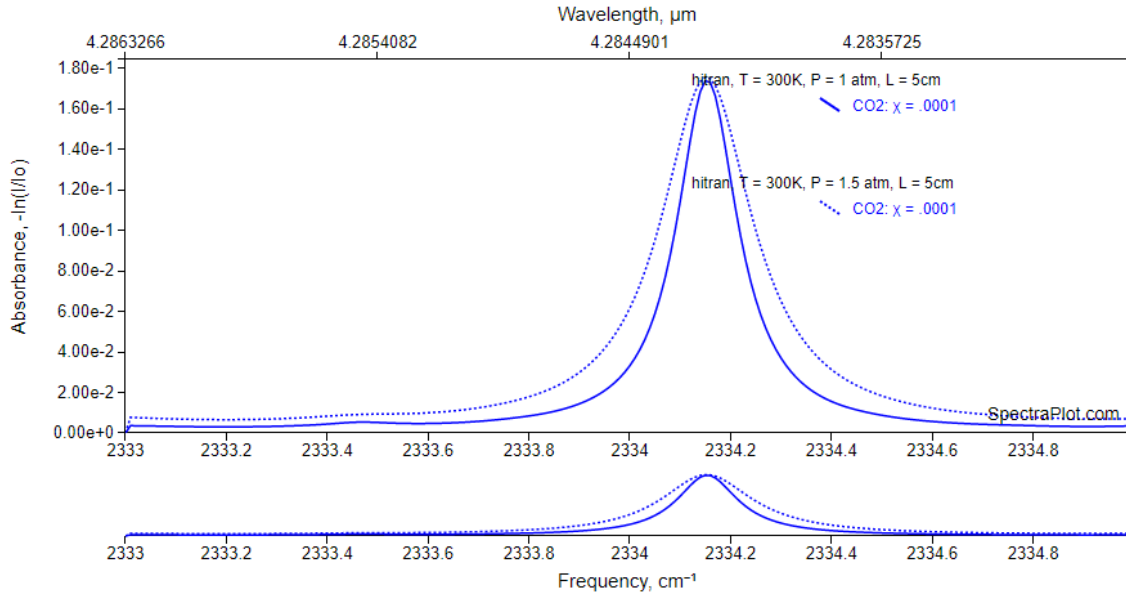
Figure 3: Absorption at 4.28μm vs. Pressure
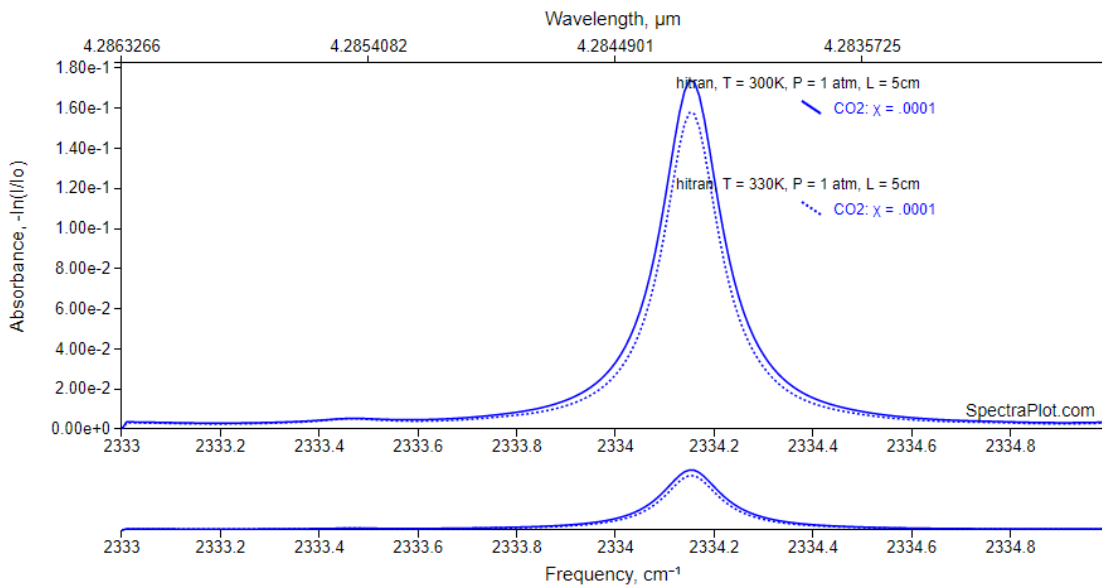
Figure 4: Absorption at 4.28μm vs. Temperature

As the gas temperature is increased, the gas molecules vibrate more intensely and increase in energy. However, the absorption of infra-red radiation actually decreases, as shown in Figure 4 by the drop in the peak and narrowing of the absorption band. This is due to a reduction in the number of gas molecules in the fixed volume that are available to absorb the IR light.

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COMPENSATION OPTIONS

It has been shown that IR radiation is affected by temperature and pressure. Depending on CO_2 measurement accuracy requirements, it may be necessary to compensate for these effects. pressure.

Temperature Compensation Techniques

Changes in temperature effect sensor accuracy in several different ways. As well as those effects that can be described by simple gas laws, the LED and photo-diode, the electronics and the mechanical parts of the sensor will be all be affected by temperature.

There are several ways to mitigate the effects of temperature on sensor accuracy. Whilst not often practicable due to cost, power, and space concerns, controlling the temperature of the sensor such as with a thermoelectric cooler (TEC) can be an effective strategy.

Alternatively, the sensor accuracy variations due to changes in temperature can be characterised and corrected.

At GSS, each sensor has built-in temperature correction based on characterisation of its behaviour over temperature and gas concentration during factory calibration.

Pressure Compensation Techniques

The impact of pressure changes on sensor accuracy depends principally on the gas concentration range to be measured. For gas concentrations below 1%, the error induced on measurement accuracy for a change in pressure of 20mbar from the nominal 1013mbar reference level is less than 2%. In most so-called ambient applications, this is below the measurement accuracy of a typical sensor and well within the required measurement limits. Therefore, typically the effects due to pressure variations on measurement accuracy are ignored for concentrations below 1%.

Above 1% concentrations, and depending on the likely variation in pressure, there is often a need to compensate for the effects of pressure on sensor measurement accuracy. Left uncompensated, measurement accuracy will be impacted by over 30%, for a 200mbar change in pressure with 100% CO_2 gas.

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APPLYING PRESSURE COMPENSATION

As discussed earlier, the shape of the absorption band changes with pressure mainly caused by increased molecule collisions. This effect is known as spectral broadening. As pressure increases, so do the number of collisions due to the higher density of molecules present, and as CO_2 has a higher density than air, there is also an effect driven by CO_2 concentration.

Ignoring the effect of spectral broadening, the measurements can be corrected for pressure based on basic gas laws. Boyle's Law states that pressure is inversely proportional to volume and is constant.

$$P1V1 = P2V2$$

If the pressure doubles, the volume must halve. This implies that for a fixed volume gas sensor, if the pressure doubles, there is twice the concentration of gas in the fixed volume of the sensor. The effects of pressure due to this basic gas law can be corrected using the following formula where P is the pressure in mbar.

$$\text{Corrected CO2 Value} = \frac{CO2\ Measurement\ Value\ from\ Sensor\ (C1)}{1 - (1013 - P)/1013}$$

This can be re-written as follows where Y (Correction Factor) is -1/1013 or -0.000987.

$$\text{Corrected CO2 Value} = \frac{CO2\ Measurement\ Value\ from\ Sensor\ (C1)}{1 + Y(1013 - P)}$$

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Figure 5 below shows how sensor measurements are affected using a constant Y correction factor. Without applying the correction, the sensor measurement would increase erroneously with increasing pressure. Including this correction factor maintains the accuracy of the measurement with changing pressure.
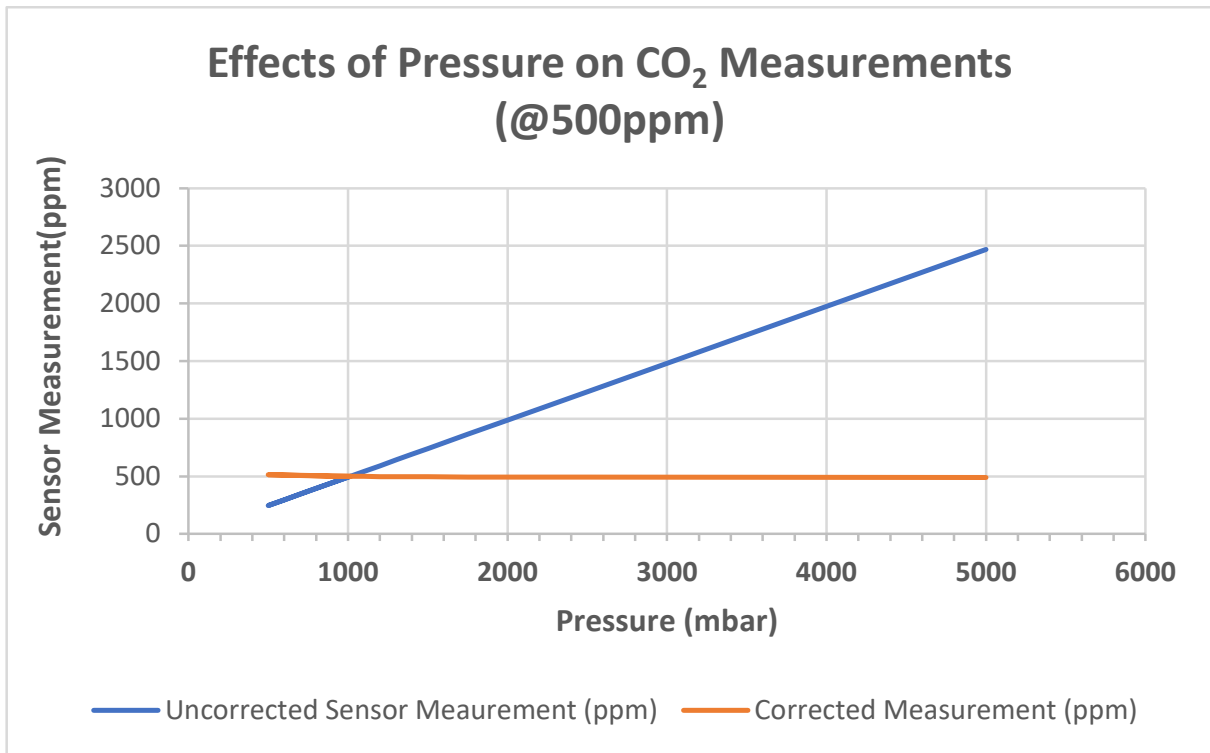

Figure 5: Effects of Pressure on Gas Concentration

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ADDING EFFECTS OF SPECTRAL BROADENING

As discussed earlier, the spectral broadening effect increases the impact of pressure as the increased concentration effect adds to the basic gas law. In the graph below, the compensation value Y combines both the spectral broadening and gas law effect to give an overall compensation value.
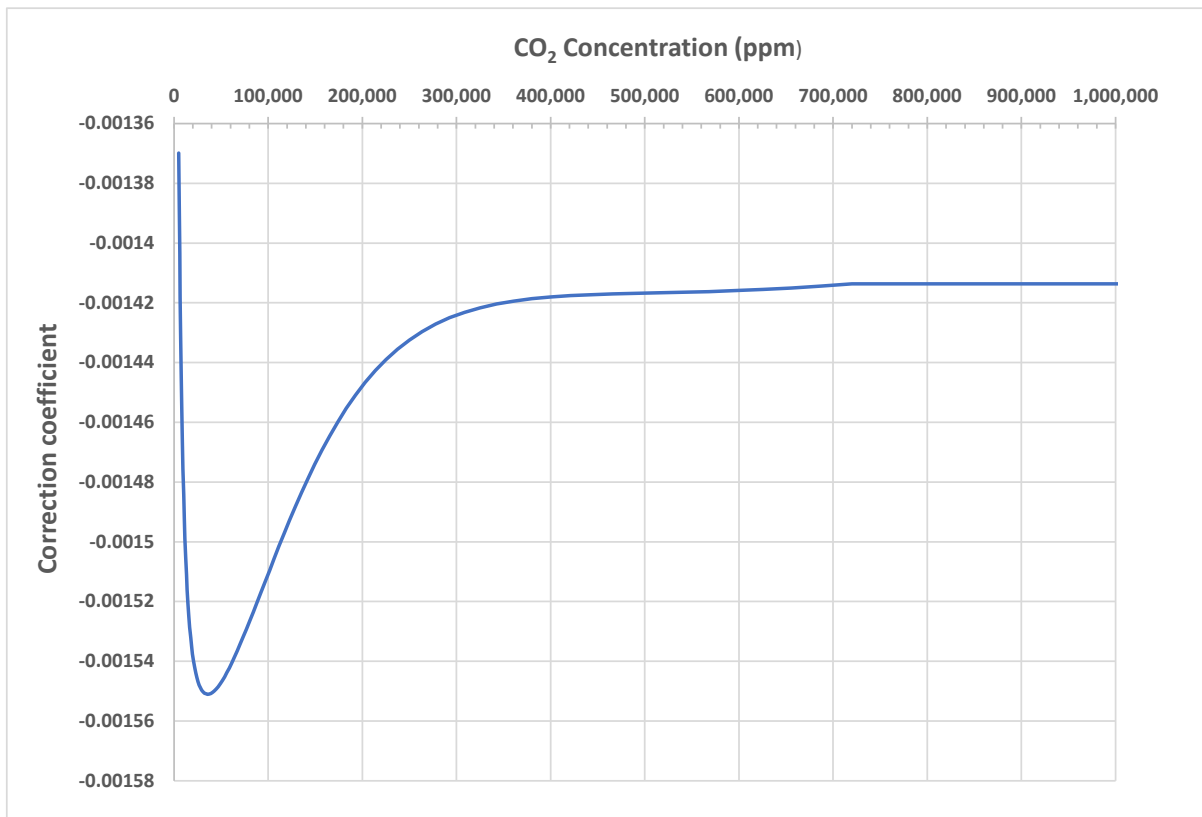
Figure 6: Correction Factor vs. Concentration

The correction factor has been derived from spectral data & confirmed experimentally. By inspection, at low gas concentrations and small variations in pressure from the nominal 1 atmosphere reference level, the impact on sensor accuracy is small.

The correction curve does not fit a simple algorithm but can be simplified for some applications depending on the concentration range to be measured. For concentrations above 30%, the coefficient can be simplified to a constant -0.0014. For other ranges, it is possible to select different coefficients depending on the range of the sensor and the nominal concentration being measured.

To improve the correction further, there are two further methods to consider. The correction factor is based on experimental data and can be used directly as part of a look up table. Alternatively, it is possible to describe the correction coefficient as a polynomial. Techniques for generating a polynomial fit are beyond the scope of this application note.

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Figure 7 below shows the best fit using a 6th order polynomial (orange line) compared to the theoretical correction coefficient (blue line).
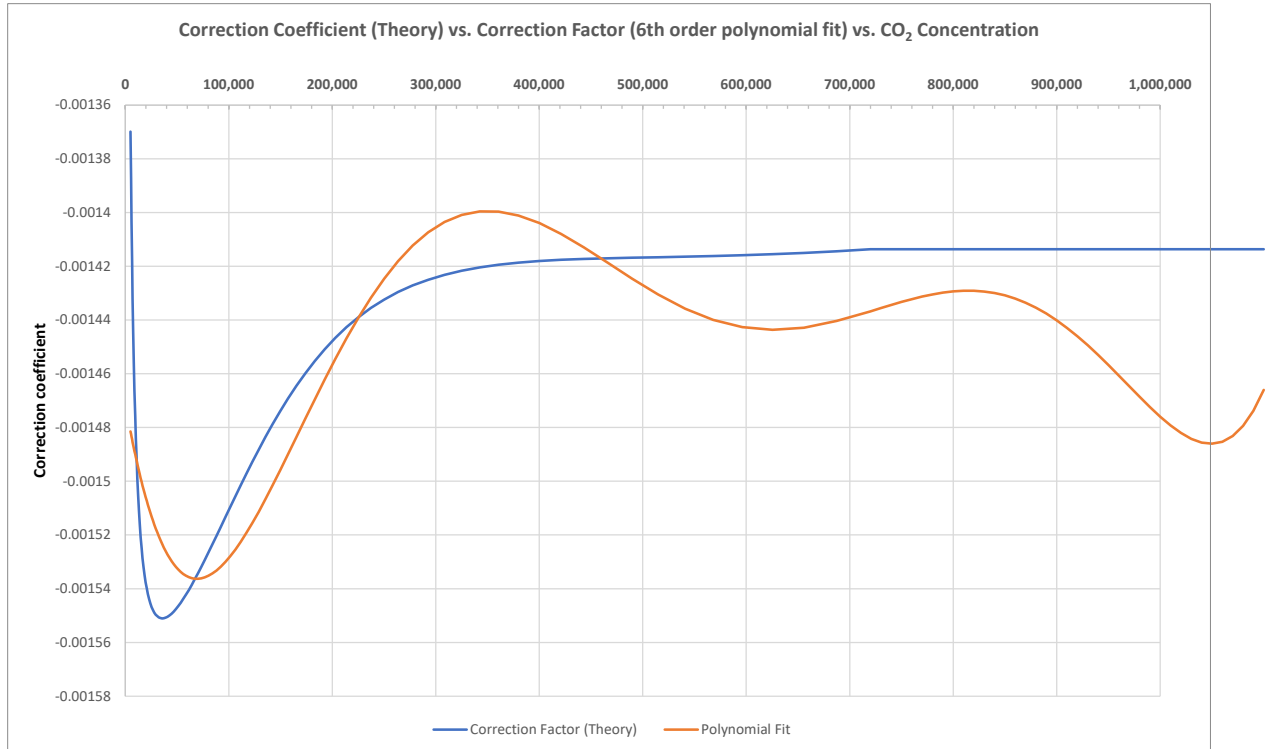

Figure 7: Correction coefficient Y

The orange line is a 6th order polynomial fit described by the following equation.

$$Y = 2.811 \times 10^{-38} x\, C1^6 - 9.817 \times 10^{-32} x\, C1^5 + 1.304 \times 10^{-25} x\, C1^4 - 8.216 \times 10^{-20} x\, C1^3 + 2.311 \times 10^{-14} x\, C1^2 - 2.195 \times 10^{-9} x\, C1 - 1.471 \times 10^{-3}$$

Other methods can be used to generate a best fit curve including using a different number of terms in the polynomial, or other non-linear regression techniques. The typical trade-off to be made is the balance between accuracy and computational complexity.

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Figure 8 below shows the impact of using the polynomial fit correction curve versus uncorrected CO_2 measurements.
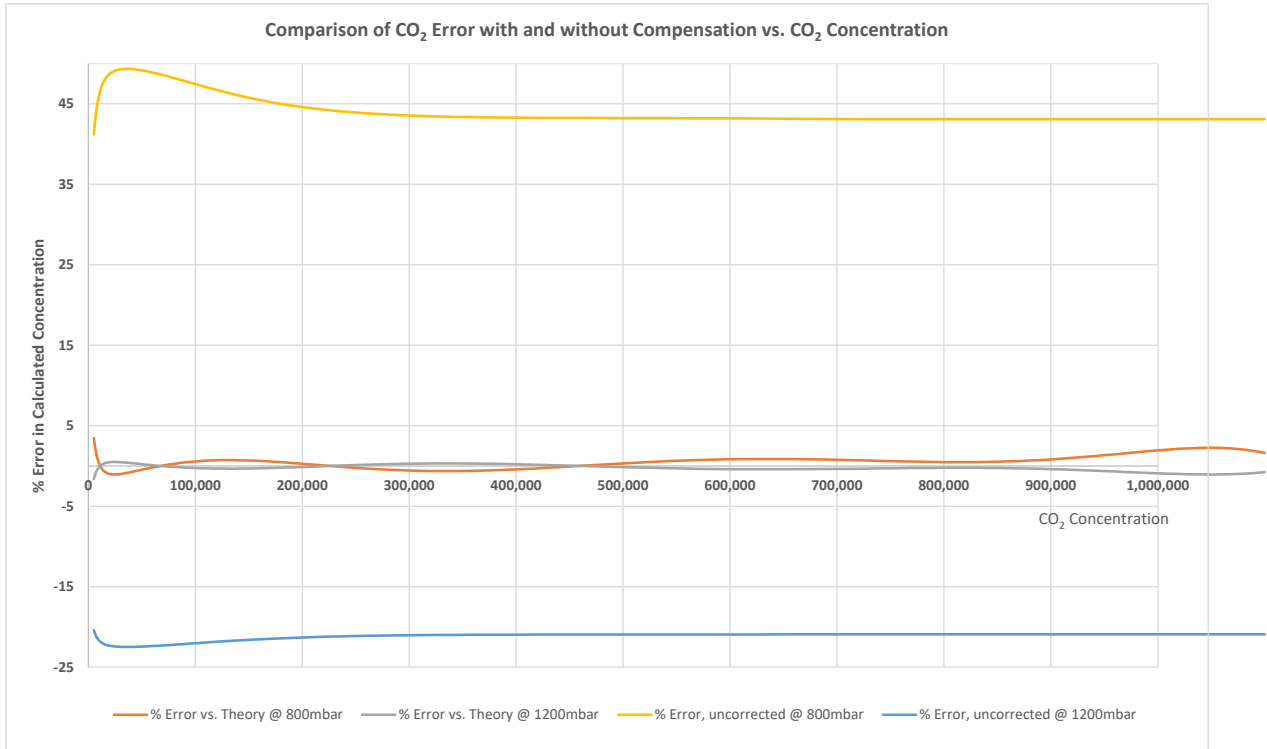
Figure 8: Comparison of Uncorrected and Corrected Measurement Errors vs. CO_2 Concentration

The corrected CO_2 measurement errors using the 6th order polynomial are typically <1% except at the extremes. This is compared to uncorrected errors of >43% for measurements at 800mbar and >20% for measurements at 1200mbar.

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CONCLUSION

Unless corrected, the accuracy of CO$_2$ measurements is compromised by the effects of ambient pressure changes, particularly at gas concentrations above 1%. This application note describes potential techniques for correcting for the effects of pressure on CO$_2$ measurement accuracy, using a constant correction coefficient, a look up table or using a polynomial fit. These techniques enable accurate pressure compensation to be applied to many different applications ranging from ambient CO$_2$ sensing to more demanding environments of up to 100% CO$_2$ concentration.

GSS can advise on the best approach to correcting errors due to changes in ambient pressure and provide detailed technical support data for each method described in this application note.

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IMPORTANT NOTICE

Gas Sensing Solutions Ltd.

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REVISION HISTORY

DATE	RELEASE	DESCRIPTION OF CHANGES	PAGES
03/05/2020	1.0	First revision	All