NDIR: Gas Concentration Calculation Overview

1. What is an NDIR Sensor?

Alphasense IRC-A sensors use the principle of Non-Dispersive Infra-Red (NDIR) to determine gas concentration. Each sensor consists of an infrared source, optical cavity, dual channel detector and internal thermistor. Gas diffuses into the optical cavity. Light from the infrared source passes through the optical cavity where it interacts with the gas before impinging on the detector. Certain gases absorb infrared radiation at specfic wavelengths (absorption bands). The dual channel detector is comprised of an active channel and a reference channel. The active channel is fitted with a filter such that the only light with a wavelength that corresponds to an absoption band of the target gas is allowed to pass through. If the target gas is present in the optical cavity the intensity of light passing through the filter and hitting the active channel decreases. The reference channel of the detector is fitted with a filter that only allows wavelengths of light where there are no absorption bands to pass through. The intensity of light hitting the reference channel is not affected by the presence of gas. The use of a reference channel allows variations in the light intensity to be compensated for. The detectors used are highly sensitive to the ambient temperature and so it is necessary to constantly monitor the temperature and compensate the output. The internal thermistor is used for this purpose.

2. How do I get useful signals from the sensor?

Full details are given in Application Note AAN 202. Briefly, in order to get useful signals from the detector in an NDIR sensor the infrared source is typically pulsed on and off at 1 to 3 Hz in a square wave, 50% duty cycle. Suggested frequencies are 2 Hz for IRC-A1 sensors which use pyroelectric detectors and 3 Hz for IRC-AT sensors which use thermopile detectors. The actual frequency is not hugely important but it must be stable. Using suitable circuitry this generates approximately sinusoidal detector output signals from a preamplifier. It is the peak to peak amplitude of these signals that is important. In the following discussion the use of active and reference signal refers to the amplitude.

3. Calibrating the sensor

For sensor calibration two parameters are needed. These are ZERO and SPAN:

ZERO. This is the ratio of the active to reference signals in the absence of the target gas:

$$ZERO = \frac{ACT_0}{REF_0}$$

where: ACT_0 and REF_0 are signals in zero gas.

ZERO is a sensor specific parameter and should be determined whenever the sensor is installed (or reinstalled) in an instrument.

The sensor should be powered on and left to warm up for at least 30 minutes in zero gas. The active and reference signals should then be measured and ZERO determined. The temperature should also be measured and recorded.

SPAN. This the proportion of radiation that impinges on the active element of the detector that has the ability to be absorbed by the target gas. Due to filter bandwidth and fine structure in absorption spectra there will be radiation that cannot be absorbed by the target gas (see Application Note AAN 204). SPAN can be determined as follows:

$$SPAN = \frac{ABS_x}{1 - \exp(-bx^c)}$$

where: ABS_x is the absorbance (see below) at the calibration concentration

X: see Table 1 for recommended SPAN concentrations for each sensor range

b and c are linearisation coefficients (see Table 1 and Application Note AAN 203).

4. Determination of Absorbance

Absorbance is defined as (see Application Note AAN 204):

$$ABS = 1 - \left(\frac{I}{I_0}\right)$$

where: I = ACT/REF

I_0 = ACT_0/REF_0 = ZERO

Absorbance can therefore be determined from the sensor outputs using:

$$ABS = 1 - \left(\frac{ACT}{REF \times ZERO}\right)$$

where: ABS_x is the absorbance (see below) at the calibration concentration

X: see Table 1 for recommended SPAN concentrations for each sensor range

b and c are linearisation coefficients (see Table 1 and Application Note AAN 203).

5) Determination of Gas Concentration

The gas concentration is determined from the following equation:

$$x = \left[\frac{\ln\left(1 - \frac{ABS}{SPAN}\right)}{-b}\right]^{\left(\frac{1}{c}\right)}$$

where: ABS is the absorbance

SPAN is the proportion of absorbing radiation (determined during calibration (see above))

b and c are linearisation coefficients (see Table 1 and Application Note AAN 203)

Note that the above equation assumes a positive absorbance. If the absorbance is negative the following equation should be used. Note that although negative absorbances imply a negative gas concentration they may be encountered due to temperature effects.

$$x = -\left\{\left[\frac{\ln\left(1 + \frac{ABS}{SPAN}\right)}{-b}\right]^{\left(\frac{1}{c}\right)}\right\}$$

6. Temperature Compensation

The effects of temperature on an NDIR sensor are complex and care must be taken to ensure effective temperature compensation. Changes in temperature affect the absorbance, SPAN and apparent gas concentration. The complexity of temperature compensation algorithms applied to the data depends on the accuracy required. Details are given below for two simple linear corrections. For details of more complex corrections to improve accuracy, users are encouraged to contact Alphasense.

6.1 SPAN ONLY compensation

For sensors with high full scale values (e.g >10 % vol. CO_2) it is normally sufficient to correct only the SPAN, using the following equation:

$$SPAN_T = SPAN_{cal} + \beta_o (T - T_{cal})$$

where: $SPAN_T$ is the SPAN at temperature, T
$SPAN_{cal}$ is the SPAN determined during calibration
β_o is the SPAN ONLY correction coefficient (see Table 1 and Application Note AAN 203)
T_{cal} is the calibration temperature

6.2 ABS AND SPAN compensation

To ensure accuracy at low concentrations, it may be necessary to correct both the absorbance and the SPAN. The absorbance is corrected using the following equation:

$$(1 - ABS_T) = (1 - ABS)(1 + \alpha(T - T_{cal}))$$

where: ABS_T is the temperature corrected absorbance at temperature, T
ABS is the uncorrected absorbance
α is the absorbance correction coefficient (see Table 1 and Application Note AAN 203)
T_{cal} is the calibration temperature

SPAN is then corrected as above but **to ensure accurate compensation a different coefficient should be used** (see Application Note AAN 203):

$$SPAN_T = SPAN_{cal} + \beta_A (T - T_{cal})$$

where: $SPAN_T$ is the SPAN at temperature, T
$SPAN_{cal}$ is the SPAN determined during calibration
β_A is the ABS AND SPAN correction coefficient (see Table 1 and Application Note AAN 203)
T_{cal} is the calibration temperature

7. Calculating the temperature corrected gas concentration

Following correction of ABS and/or SPAN, the gas concentration can be calculated. However, in order to relate the gas concentration (in % volume) at temperature, T, with the gas concentration (in % volume) at the calibration temperature it is necessary to employ the ideal gas law. This accounts for apparent changes in the gas concentration with temperature (because an NDIR sensor is sensitive to the number of molecules of the target gas in the cell, not the % volume) so that the gas concentration at temperature, T, is given by:

$$x_T = \left[\frac{T}{T_{cal}}\right]\left\{\left[\frac{\ln\left(1 - \frac{ABS_T}{SPAN_T}\right)}{-b}\right]^{\left(\frac{1}{c}\right)}\right\}$$

8. Summary of Coefficients

Table 1. IRC-A1 : Standardised Linearisation and Temperature Compensation Coefficients (assuming calibration at 20°C)

Sensor	Gas	Range (SPAN Conc.)	Linearisation Coefficients		Temp. Comp. Coefficients		
			b	c	β_O	α	β_A
IRC-A1-IAQ	CO_2	0 to 5000 ppm (4000 ppm)	4.1×10^{-4}	0.897	N/A	0.0009	0.0005
IRC-A1-Safety	CO_2	0 to 5 % Vol (4 % Vol)	0.520	0.680	0.0021	0.0009	0.0014
IRC-A1-Combustion	CO_2	0 to 20 % Vol (16 % Vol)	0.491	0.613	0.0024	0.0009	0.0020
IRC-A1-Industrial	CO_2	0 to 100 % Vol (100 % Vol)	0.698	0.302	n.d	n.d	n.d

Table 2. IRC-AT : Standardised Linearisation and Temperature Compensation Coefficients (assuming calibration at 20°C)

Sensor	Gas	Range (SPAN Conc.)	Linearisation Coefficients		Temp. Comp. Coefficients		
			b	c	β_O	α	*β_A
IRC-A1-IAQ	CO_2	0 to 5000 ppm (4000 ppm)	3.25×10^{-4}	0.9363	0.00001	0.00056	0.00001
IRC-A1-Safety	CO_2	0 to 5 % Vol (4 % Vol)	0.5411	0.6716	tbd	0.00056	tbd
IRC-A1-Combustion	CO_2	0 to 20 % Vol (16 % Vol)	1.0459	0.2932	tbd	0.00056	tbd
IRC-A1-Industrial	CO_2	0 to 100 % Vol (100 % Vol)	tbd	tbd	tbd	tbd	tbd