

Application Note DESA3: Infrared Gas Sensor General Notes

Electromagnetic radiation encompasses a huge range of wavelengths from long wavelength, low energy, radio waves to extremely short wavelength, high energy, gamma rays. The infrared region of the spectrum generally covers the wavelength range 700nm out to 1mm and within this range the 3 – 10 micron wavelength region is of interest as it interacts with certain chemical bonds and provides a means of detecting molecules. Molecular bonds vibrate and bend in relation to each other, effectively oscillating. If these oscillations produce a change in dipole moment then they can absorb electromagnetic radiation tuned to those oscillations and this tends to occur in the infrared region. Stretching of bonds tend to have fundamental absorbances in the 3-5 micron region whereas weaker bending modes tend to have absorbance in the 5-10 micron region and beyond.

Carbon dioxide as an example is a linear triatomic molecule and the two C=O bonds can stretch symmetrically or asymmetrically:



The symmetric stretch does not produce a change in dipole moment and is therefore not infrared active. However, the asymmetric stretch does produce a change in dipole moment and so is infrared active. The asymmetric stretch absorbs infrared radiation in the 4.2 - 4.45 micron wavelength region resulting in a spectrum as shown:



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By measuring the intensity of radiation in the wavelength range absorbed by the asymmetric stretch it is possible to determine the amount of gas present. The more gas is present, the more radiation is absorbed. An infrared gas sensor comprises a radiation source and a radiation detector housed within an optical arrangement into which target gas diffuses. A simplistic example is shown below:



Gas diffusing into the path of the radiation absorbs wavelengths of IR radiation, which is monitored by the detector. The more molecules there are between the source and the detector the greater the amount of absorption. The number of molecules in the path increases with pathlength and with the gas concentration. So for a fixed pathlength it is possible to measure the gas concentration by measuring the amount of target radiation absorbed.

The radiation detector is often a dual detector containing 2 detector elements that respond to radiation emitted by the radiation source. One detector element (the active) responds to radiation of wavelengths emitted by the radiation source that are absorbed by the target gas. The other detector element (the reference) responds to radiation emitted by the radiation source that is not absorbed by target gas. The radiation detector therefore provides an active signal (affected by target gas) and a reference signal (unaffected by target gas). The reference signal is used to compensate for changes in radiation intensity caused either by the radiation source (e.g. through ageing) or by changes in the optical characteristics of the optical arrangement (e.g. through neutral density contamination).

The radiation detector can be a pyroelectric detector that responds to <u>changes</u> in incident radiation, unlike a photometric detector that responds directly to incident radiation. Also for thermopile and other types of detector the radiation is often chopped in order to generate changes in incident radiation at the detector, providing a white and dark space signal. This chopping is achieved by pulsing the radiation source, which is often a low power filament lamp but can also be a thin film black body emitter or an LED. The source is typically driven by a square wave supply, which should be of a constant frequency and ideally a constant 50% duty cycle. Typical operating frequencies are in the range 2.0Hz - 10.0Hz, where detector responses are close to optimum, although some LED sources are chopped at faster frequencies and smaller duty cycles.



The detector signals typically comprise a DC voltage pedestal upon which is superimposed a small oscillating signal in sympathy with the lamp chopping. Therefore a low frequency AC amplifier is typically used to extract the sensing signals from the DC voltage. It is important that the preamplifier gain be optimised for the frequency range of the lamp chopping. If the preamplifier AC response is optimised at higher frequencies then some differentiation of the signals occurs and this shows itself as a distortion in the signals. Ideally the signals should have a sinusoidal shape. Any differentiation will show as a peak response decaying to a lower value before the next half cycle occurs. The larger the difference between the preamplifier frequency response and the chopping frequency the more this decay and distortion appears.

In the presence of target gas the active oscillating signal reduces as the target gas absorbs radiation detected by the active element, whereas the reference oscillating signal remains constant. In order to accurately monitor the signals there must be some amplification of the small oscillating signal without amplification of the DC voltage pedestal. The resulting signals can then be read directly via an A/D converter for example and used to obtain a measure of the target gas concentration.

In order to compensate for changes in incident radiation and temperature it is normal to use the ratio of the active (gas responding) signal to the reference (non-gas responding) signal. This ratio can be based on peak-to-peak values, integrated areas or FFT amplitudes. Whichever method is used, the absorbance can then be defines as:

Absorbance = 1 - active / (zero * reference)

Where zero is the ratio of active to reference signals in zero target gas (e.g. nitrogen).

As gas enters the pathlength, the active signal reduces and therefore the ratio of active to reference signal reduces and the corresponding absorbance rises. The relationship between the absorbance and gas concentration is nonlinear as illustrated in the following absorbance curve plots:



For a single wavelength the Beer-Lambert Law can be applied to describe the non-linearity:

 $I = I_0 e^{(-cl)}$ in intensity terms and $(1 - I/I_0) = (1 - e^{(-lc)})$ in absorbance terms

where I is the signal intensity (e.g. active signal), I_0 is the signal intensity in the absence of target gas, is called an extinction coefficient which is a function of the wavelength and the spectrum of the target gas, c is the gas concentration and I is the pathlength.

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However, for signals based on pass band optical filters (where more than one wavelength is being monitored) this relationship is modified because we are looking at a range of different wavelengths with a corresponding range of different extinction coefficients. Looking at the CO_2 spectrum above for instance, some wavelengths are not absorbed at all whereas adjacent wavelengths are strongly absorbed. It has been found empirically that this deviation can be defined using the following modified relationship in absorbance terms:

$$(1 - I/I_0) = s(1 - e^{(-(c^n))})$$

where s corresponds to a span factor (i.e. a measure of sensitivity), is an exponential constant related to the extinction coefficient and pathlength, c is the gas concentration and n is a power term applied to the gas concentration. Such a treatment provides an excellent fit to the observed absorbance curves above.

Different gases have different spectra and different extinction coefficients. In the case of hydrocarbons, the generic C-H bond stretch is commonly viewed as the fundamental range to monitor. There are strong differences between methane and heavier hydrocarbons as illustrated in the spectra of methane and ethane below:



Methane shows discrete lines of absorbing wavelengths whereas ethane shows a more continuous band. The overall total absorbance of methane in the 3.15 - 3.5 micron range is much lower than that for ethane since the methane spectrum has many gaps in the absorbance band. Sensors that monitors for methane using a typical methane optical filter as shown will therefore respond strongly to the presence of ethane and also to other hydrocarbons.

Where there are gas mixtures, the combined response is therefore a combination of the response to different gases in the mixture. For a methane sensor calibrated in %volume methane terms, exposure to a mixture of methane and a small amount of ethane will read noticeably high on the methane scale because of the ethane response. Since the absorbance characteristics are not linear, the effect is not simply additive so is difficult to compensate. Unless a special sensor is used, cross interference on methane can cause high readings in gas mixtures containing methane and other hydrocarbons.

In %lel terms the PrimePell has fairly similar responses to similar lels of target gases, due partly to the custom optical filters used. For example a PrimePell calibrated to %lel methane and exposed to %lel butane will read the butane level reasonably accurately up to at least 50%lel. This is a significant benefit for the PrimePell since other IR sensors commonly read very high under these conditions, small levels of butane overloading the range.



For combustible gas mixtures the lel (lower explosive limit) of the gas mixture is a function of both the lel of the component gases and the amount of each component present. Le Chetalier's principle is typically used to calculate the lel of the mixture:

lel = 100/(x1/L1 + x2/L2 + ... xn/Ln) %(vol)

where:

lel = lower explosive limit of the gas mixture (% volume in air)Li = lower explosive limit of component i (% volume in air)xi = concentration of component i in gas mixture (% volume in air)

So if we consider a mixture consisting of 70% methane (lel = 5% volume) and 30% ethane (lel = 2.5% volume) the lel of the mixture in air is given as:

lel = 100/(70/5 + 30/2.5) = 3.85% volume

Note that in oxygen enriched or partially inerted (oxygen depleted) atmospheres these levels change. Also, a minimum amount of oxygen is required for complete combustion but an infrared sensor does not require the presence of oxygen to detect target gas. A Prime1 calibrated for %volume methane or a PrimePell calibrated for %lel methane will still respond the same to hydrocarbon gases irrespective of the amount of oxygen present.

So for gas mixtures we not only have a change in the linearity and sensitivity of a sensor compared to a single target gas but we also have a change in the explosive limit of gas mixtures. Care must therefore be taken to consider the worst case when considering sensor calibration or alarm set points.

This mixture problem does not apply to sensors that respond to gases that do not have common interference caused by overlapping spectra. For example, for a CO_2 sensor such as a Prime2 or a Prime3 the absorbance of CO_2 is strong and there is little response to other gases in the same spectral region. CO does have some absorbance close to one of the CO_2 bands but it is a weak absorber and does not have a very significant effect. For acetylene there is a possible interference by water vapour overlap although the Prime4 sensor shows very little interference due to its special optical components.

Infrared sensors are molar sensors, in other words they monitor the molar concentration of gas in the optical cavity. The molar concentration is covered by the ideal gas law so for a given %volume concentration the molar concentration increases with increasing pressure and reduces with increasing temperature. The ideal gas law effect for temperature can be included within the Prime configuration but for pressure there is no internal pressure sensor. Therefore a sensor calibrated at one pressure will read high in a higher pressure and low in a lower pressure. Again, because of the non-linear nature of the response this is not something that can be linearly compensated very well. Care should be taken when calibrated at the surface of a mine and then taken underground will experience a pressure increase while underground and therefore the instrument is likely to read high when in use unless it is calibrated underground at the mine pressure, despite the fact that temperature generally increases with depth which would tend to reduce the reading; however, Prime sensors are temperature compensated so the temperature effect is a lot smaller than the pressure effect.

Since infrared sensors are optical sensors care has to be taken to avoid problems caused by water condensation within the optical arrangement. Prime sensors do self-heat internally so the temperature within the optic is typically 10'C higher than the ambient temperature; this helps to avoid condensation inside the optical path. Where a sensor is likely to be used in a condensing situation it is normally good practice to use a water barrier, typically a PTFE membrane, across the face of the sensor to prevent liquid water entering the sensor. A typical application would be for monitoring biogas where the humidity is very high, the sample temperature is often significantly above external ambient and the method to allow the gas to reach the sensor has to be carefully considered. For example, if gas were sampled and blown directly at the face of a sensor then high humidity and possible liquid water are forced directly at the face of the sensor. A PTFE membrane could stop the liquid water but not everything else. In such a case it is better to flow gas across the face of the sensor not directly at the face.



One should also consider condensation in the flame arrestor section of a sensor. Even with a PTFE membrane, water vapour can still cross to enter the sensor and depending on the environmental conditions the flame arrestor area can be the coolest part of the gas path within the sensor. Care should be taken because if water condenses within the flame arrestor then it can effectively block the flame arrestor and prevent gas entering the sensor. In this situation a gas sensor would not be responding correctly to the gas in its surroundings.

If sufficient condensation were to occur within the optical path then the radiation reaching the detector elements can reduce significantly and not evenly. This can result in a significant shift in the output and ultimately detector signals that are too low. The Prime sensors have an extensive fault monitoring system and if the signals are too low (either active, reference or both) a fault is triggered and the output voltage goes to the fault level. The serial interface can be used to gather information as to the cause of the fault if required. For example, if both active and reference signals collapse then it could be that the IR source has failed, the IR detector has failed or the optical path has been obscured.

Certain faults are recoverable and if the Prime sensor is in such a fault state and that condition resolves itself then the Prime sensor will recover.

A typical example is if the supplied voltage drops below the 3.0V threshold. If the voltage supply was too low the Prime sensor will detect it and go into fault mode but if the supply voltage level rises again then the Prime sensor will detect that and restart. It is important to note that although once up and running the Prime sensor consumes a fairly constant current level of approximately 75mA there can be an initial inrush current during the first start-up period. If the power supply to the sensor does not have enough current capability then the voltage supplying the sensor can drop below the minimum threshold and the sensor may fail to start. It is recommended that at least 130mA be available to cater for the initial inrush current.

If the analogue output were to be affected by an external condition (e.g. a short circuit or a voltage being applied to it) then the Prime sensor will also detect that the voltage output is not what it should be and go into fault mode. If the affect on the output is removed and no damage has been done then the Prime sensor will restart automatically.

Every hour the Prime sensor enters a self-test mode for a very short period. During this mode it tests the integrity of the internal memory, program, data, supply voltage, internal voltages, reference voltages and ADC operation validity. If any error is detected then the Prime sensor will go into the fault condition, again the serial interface can be used to obtain more information. Most of these internal faults are fatal but a continuous check is made and if they are recoverable then the Prime sensor will restart automatically.

A special feature of the Prime sensors is that they operate independent of the supply polarity. This is a design feature to enable operation in a pellistor mode where the output of the sensor mimics a pellistor bridge signal. If the polarity of the supply voltage is positive on the detector supply pin and negative on the compensator supply pin then the output is mid supply at zero gas and reduces in the presence of gas, as does a pellistor. If the polarity of the supply voltage is negative on the detector supply pin and positive on the compensator supply pin then the output is mid supply at zero gas and increases in the presence of gas, as does a pellistor. When a Prime sensor is providing a voltage output (typically 0.4V at zero gas and 2.0V at full scale gas) the output voltage automatically relates to the negative side of the supply. So there is no need to stock different supply polarity versions.

Another special feature of the Prime sensors is the algorithms used to extract the signals from the detectors. Infrared sensors typically operate with a switched source, typically the source is turned on and off at low frequency (between 1Hz and 10Hz) and this means low frequency AC amplification is used between the detectors and the A/D converter. For ranges that are very sensitive, small amounts of AC noise can make quite a difference to the resulting concentration so it is typical to use various filtering methods to dampen noise from cycle to cycle. The Prime sensors use an advanced Fast Fourier Transform technique to optimise the signal readings from the detectors coupled with advanced filtering methods that allow the sensor to operate at the higher frequency range (typically 8Hz) and use over sampling methods to further assist in noise reduction.

The Prime sensors also have an extensive serial interface that allows interrogation and modification of the configuration to suit special applications. It is important to note that any changes to the configuration can affect the output signals and care must be taken to ensure that the integrity of the sensor is maintained and that the response is correct for the application. It is not recommended that the configuration be adjusted without due care. Changing the configuration does not normally affect the temperature compensation on the zero but changing the range is likely to affect the temperature compensation for the span.



The flexibility of the Prime sensors enables the same sensor type to be configured for a wide range of applications. For example, a Prime2 sensor can be configured for CO_2 ranges as low as 0-2000ppm and as high as 0-10% volume. A PrimePell or a Prime1 can be configured for ranges from 0-10000ppm methane up to 0-100% volume methane. This flexibility enables the use of Prime sensors in many wide and varied applications without the need for special sensor variations, all the changes are made within the configuration. Prime sensors are supplied precalibrated to the range required and temperature compensated for that particular range.

The Prime sensors can be recalibrated using the serial interface commands. As with any calibration, it is important to establish the zero calibration first and then the span gas calibration. It is normal to flow calibration gas (both zero and span gas) across the face of the sensor to allow the gas to diffuse into the sensor through the flame arresting mesh. A typical calibration gas flowrate is between 500ml/min and 1 litre/min. Note that pressure build-ups should be avoided as the sensor is a molar sensor and although the zero will not be affected by pressure the span calibration will be affected. The higher the pressure the higher the reading in gas.

For CO₂ sensors in particular, ambient air must not be used as a zero gas. Ambient fresh air typically contains approximately 500ppm of CO2 and people breath out typically 5% CO2 so it must be stressed that performing a zero calibration on a CO₂ sensor in ambient air with people breathing nearby is not correct. A room with people inside can easily reach a background level of 1000ppm with little ventilation so the zero calibration should be carried out in CO₂ free gas, typically nitrogen but CO₂ free synthetic air is also acceptable.

Generally it is advisable to calibrate at or near the top of the concentration range where possible. This is because the zero point and the span calibration point are then fixed and points in between generally have better linearity than points extrapolated above the concentration range. For example, a PrimePell calibrated for 0-100%lel methane with the span calibration carried out at full scale will hold linearity to typically within 1-2%lel across the range. If the sensor were calibrated at 50% lel then concentrations above that calibration point are extrapolated and a small error at 50%lel could mean the full-scale reading at 100%lel could deviate by 3-5%lel. For high resolution sensors such as the Prime1 or PrimePell set for 0-100%volume methane high resolution or a Prime3 set for 0-100%volume CO2 there are actually 2 span calibration points, one to cater for the lower range and provide the high resolution and one for the higher range to cater for the linearity over the full scale.