Infrared Sensor Application Note 1
A Background to Gas Sensing by Non-Dispersive Infrared (NDIR)

INFRARED GAS ABSORPTION SPECTRA

It is well known that many gas molecules can absorb radiation in the infrared portion of the electromagnetic spectrum. When infrared radiation is incident on the gas, the energy states of atoms vibrating in the molecules change in discrete steps when the wavelength of the infrared matches the molecules natural frequencies or resonances. Put simply, the vibrations of atoms held in their chemical bonds increase when excited by light of the right wavelength. A net absorption of infrared radiation effectively raises the gas temperature.

The resonant frequencies (wavelengths) depend on the number and masses of atoms in the molecules as well as the number and strengths of the various chemical bonds. If the chemical structure of the molecules is complex, then there will be a whole range of resonant vibrations. This is often presented graphically as a series of absorption peaks plotted against wavelength, called an absorption spectrum. A few gas absorption spectra are shown in Figs 1 to 7. More can be found by viewing the NIST chemistry web book at http://webbook.nist.gov/chemistry/

IR interacts with the gas only if it 'sees' a dipole on the molecule (an analogy is radio waves picked up by an aerial). Molecular dipoles exist if atoms in the molecules are arranged non-symmetrically or if the modes of vibration are non-symmetrical. The vibrations include stretching and bending of the molecules that distort them to create dipole or even multi-pole moments. This is illustrated in Fig 8 for CO_2.

It is worth noting that rotational energy states for gas molecules also exist, but these tend to be excited by much longer wavelength radiation in the microwave region.

Symmetrical molecules, such as the binaries H_2, N_2 and O_2, are not excited by IR because their structures and modes of vibration do not create any net dipoles.

Carbon dioxide is a good example of a symmetrical molecule that has symmetrical and non-symmetrical modes of vibration (Fig.8) so it absorbs IR.

Other gases and vapours, especially hydrocarbons are active in the IR largely through C-H stretching modes. Generally the greater the number of C-H bonds, the stronger the absorption lines, many of which merge into bands.

DISPERSIVE INFRARED

IR gas absorption spectra cover a wide range from 2.0 to 20 microns and show a multiplicity of broad peaks and fine line structures. These features are characteristics of the gases, rather like individual fingerprints. Their wavelength positions enable the gases to be identified, while their heights provide information from which the gas concentrations may be calculated.

An instrument required to plot spectra of this type is generally known as 'dispersive', because IR passing through the gas is then split or 'dispersed' into the spectrum by a diffraction grating, a prism or perhaps a tuneable filter before entering a suitable detector. It is really a gas spectrometer. Most dispersive IR instruments are very expensive, bulky and somewhat fragile bench-top systems which are usually confined to laboratories. Unfortunately they cannot easily be used to identify and continuously monitor gases in real field applications. Hence very few dispersive IR gas-sensing systems are deployed in hazardous locations.

NON-DISPERSIVE INFRARED (NDIR)

For the majority of IR gas sensing applications, the identities of the target gases are already known, so there is little need for gas spectrometry. The user must still measure the concentration of the target gas, but may be able to accept a certain degree of cross-sensitivity between different gases, if their absorption lines overlap. A Non-Dispersive Infrared sensing technique is more suited to these basic requirements.

For NDIR it is usual to regard the sensor as an individual component in the instrument. The key feature is that fixed narrow-band filters are used with individual IR detectors to identify a few gas absorption lines over a limited wavelength range. (This cuts out the dispersive part of a gas spectrometer). Relatively inexpensive sensor components can be resourced and smaller more rugged sensor packages can be fitted into instruments. The simplicity of design makes it easy for the sensor package to meet certifiable safety standards. Furthermore, gas concentrations can be derived in real time from simple algorithms used in the instrument's microprocessor.

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Choice of Sensing Wavelengths

This is governed by the available output range of IR sources and the need to work within the ‘water windows’. The water absorption spectrum in Fig. 1 shows strong absorptions below 3 microns, between 5 and 8 microns, and beyond 16 microns. Any attempt to sense gas spectral lines in these regions would be subject to strong interference if humidity were present with the target gas. Therefore it is safer to operate in either the 3 to 5 micron or 8 to 16 micron windows where many useful gas lines exist. The 3 to 5 micron window is chosen because:

- There are useful absorption lines at 4.2 microns for CO_2 sensing and at 3.0 to 3.5 microns for hydrocarbon sensing. See Figs. 2 to 7.
- There are no gas absorption lines at 4.0 microns, enabling a reference signal to be taken at this wavelength.
- IR lamps with glass envelopes radiate to 5 microns.

Gas sensing in the region beyond 8 microns is less popular as it requires an expensive IR source with a specialised IR transmissive and sealed window. The radiation from an incandescent filament also falls away at longer wavelengths. Moreover, there are no low cost solid-state IR sources commercially available at long wavelengths.

The Beer-Lambert Law for NDIR Gas Absorption

Fig. 9 shows a generic set up for sensing gas by NDIR, comprising:

- Absorption cell with reflective surfaces and gas admission.
- IR source, typically a small tungsten filament with glass envelope.
- IR active detector, typically a pyroelectric packaged with a narrow bandpass filter tuned to the target gas.
- IR reference detector with neutral (4 micron) filter for background monitoring.

Power supplies and electronics for processing signals are not shown.

Pyroelectric detectors respond to changes in light level, so the IR source has to be modulated. This can be done with a mechanical chopper wheel, but it is preferable to have no moving parts and pulse the filament voltage with square waves. At a pulse rate of 1 to 10 Hz the output of the detectors is sinusoidal with a peak-to-peak AC voltage proportional to the intensity of the IR incident on the detector. In the event of an IR-absorbent gas entering the cell, the IR intensity on the active detector will decrease according to a simple exponential relationship called the Beer-Lambert Law:

$$\mathbf{I = Io\ exp(- K\ L\ C)} \text{ .... } \mathbf{(1)}$$

Where:

I	is the intensity in target gas
Io	is the intensity in zero gas, e.g. nitrogen.
K	is a factor dependent on the gas absorption lines and the band- width of the filter
L	is the optical path-length between lamp and detectors
C	is the concentration of the gas

From (1) it is apparent that the gas concentration C can be determined.
For the active detector output there is a corresponding output voltage change, where:

$$\mathbf{(Vo - V) / Vo = (Io - I) / Io} \text{ .... } \mathbf{(2)}$$

V	is the output in target gas
Vo	is the output in zero gas

Equation (2) is a measure of how well the ‘set up’ senses gas and is called the Fractional Absorbance (FA). (For simplicity, the reference channel is excluded).

Re-arranging equations (1) and (2) gives:

$$\mathbf{FA = 1 - exp(- K\ L\ C)} \text{ .... } \mathbf{(3)}$$

If K and L are held constant, then FA may be plotted against C as shown for example in Fig. 10. The value of FA increases with C but eventually saturates at high gas concentration. This implies that for any fixed ‘set up’ the ability to resolve a change in gas level is better at low concentrations than at high. However since K, L and C are factors, then K and L can be adjusted to give the optimum absorbance for the required range of gas concentration. As a rule: long optical paths are more suited for low gas concentrations and short optical paths are more suited for high gas concentrations. There are size and power limitations, especially for long optical paths, where IR lamp outputs may not be sufficient to produce strong enough detector signals.

For the purposes of sensing hydrocarbons to the Lower Flammable Limits (LFL) and carbon dioxide to a low % volume concentration, then selecting L to a value around 50 mm is optimum.

The Modified Beer–Lambert Law and Normalised Absorbance

It must be realised that the simple Beer-Lambert expression is idealised when it comes to applying to a practical gas-sensing device. Because of dimensional and component variances, the following points are considered:

- The optical path length L is unlikely to be a single value.
- Lamp intensity and spectral outputs can vary.
- Filter band passes and transmissions can vary from batch to batch.
- Gas line absorption factors are not single value for all wavelengths, but are averaged within the filter pass band.
- The performance of the sensor will vary with temperature and pressure (see below).

Every effort must be made to minimise these variances by ensuring a good build standard. This starts with a sensor designed to be fit-for-purpose and by using reliable components. Rigid mechanical and optical alignment is of prime importance to achieve consistent performance from sensor to sensor. Any remainder variances can be catered for by redefining the Beer-Lambert Law and Absorbance expressions and using compensation algorithms.

Two coefficients, a and n, are introduced to modify equation (1):

$$I = Io \exp(-a C ^ n) \quad \ldots\ldots (4)$$

Where a and n are fixed values dependent on a particular sensor design and target gas.

Equation (2) is rewritten as a Normalised Absorbance by introducing the reference channel:

$$NA = 1 - I / Z * Io \quad \ldots\ldots (5)$$

Where $Z = I / Io = V(ref) / V(ref)o$, that is the equivalent ratio for the reference detector.

Looking at the corresponding detector voltage outputs then (5) becomes:

$$NA = 1 - (V/Vo) * V(ref)o / V(ref) = 1 - (V/V(ref)) / (Vo / V(ref)o)$$

For simplicity, the nomenclature is redefined by stating:

$$NA = 1 - Act / (Zero \times Ref) \quad \ldots\ldots (6)$$

Where:
Act = Active signal
Ref = Reference signal
Zero = Act / Ref in zero gas

It should be noted that in equation (6) and throughout, the expression of voltage ratios removes the dependence on any absolute voltage value. This eliminates any differences in detector responsivity or amplifier gain and acts to self-compensate changes in background optical conditions.

Equation (6) is then linked to equation (1) including a gas span factor:

$$1 - Act / (Zero \times Ref) = Span (1 - \exp(-aC^n) \quad \ldots\ldots (7)$$

Equation 7 is the one used to calculate the gas concentration. It is usual for instrumentation readings to be linearised with gas concentration using an algorithm in the microprocessor.

Further details of the subsequent signal processing, including linearisation and temperature compensation, are described in Infrared Sensor Application Note 2. A method of deriving the coefficients a and n for sensor types is detailed in Infrared Sensor Application Note 5.

EFFECTS OF AMBIENT TEMPERATURE AND PRESSURE

In cases where the ambient pressure and temperature are changing, the ideal gas law must be used to calculate the gas concentration.

$C = k\,P\,V / T$, where k is a constant, P is pressure, V is volume and T is temperature in kelvin, is true for non-extreme gas conditions found in most gas monitoring applications. Simple corrections to the algorithms can be factored in, provided the instrumentation is set up with independent temperature and pressure sensors.

However, the ideal gas law cannot take into account any effects that the sensing system itself introduces. The most important effect is that of temperature in an operational range limited between –40 °C and +75 °C.

An IR gas sensor by its nature senses temperature by absorbing radiation, but it also responds to temperature changes in the ambient which can give rise to spurious and misleading signals. This happens largely through a sum of responses from individual components in the sensor that are sensitive to temperature change.

The main ones are:

- Changes in IR filter characteristics.
- Changes in the pyroelectric detector outputs.
- Changes in mechanical and optical alignment.

By selecting suitable components and ensuring consistent build standards, the sensor responses to temperature are predictable and close to linear over the range -40 to +75 °C. This makes it relatively easy to compensate for in software once the sensor characteristics are fully understood. In Infrared Sensor Application Notes 2 and 5, it is shown that only two coefficients, Alpha and Beta, are required for each of the sensor types to compensate for temperature change. This includes corrections for the ideal gas law.

A separate temperature sensor, mounted close to the gas sensor, is required to effect the compensation. Some of the e2v IR gas sensors (IR1xxx Series 2 and IR15T Series) have built-in temperature sensors.

ADVANTAGES OF NDIR COMPARED WITH CATALYTIC GAS SENSING

- It is a physical sensing technique which is unaffected by aggressive chemical environments. There are no poisoning effects as suffered by catalytic sensors.
- Gases may be sensed in anaerobic conditions, i.e. oxygen is not required for operation.
- Hydrogen is not detected and therefore causes no cross-sensitivity.
- Carbon dioxide is uniquely detectable with no interference from other gases.
- There are no problems with sensor deterioration or ‘burn-out’ if exposed to high gas concentrations or if monitoring gases for very long periods.
- Stable long-term operation requires less recalibration.
- Stable after long period of storage.
- Life expectancy exceeds 5 years, much longer than catalytic sensors.
- Cost of ownership is low compared with catalytic sensors.

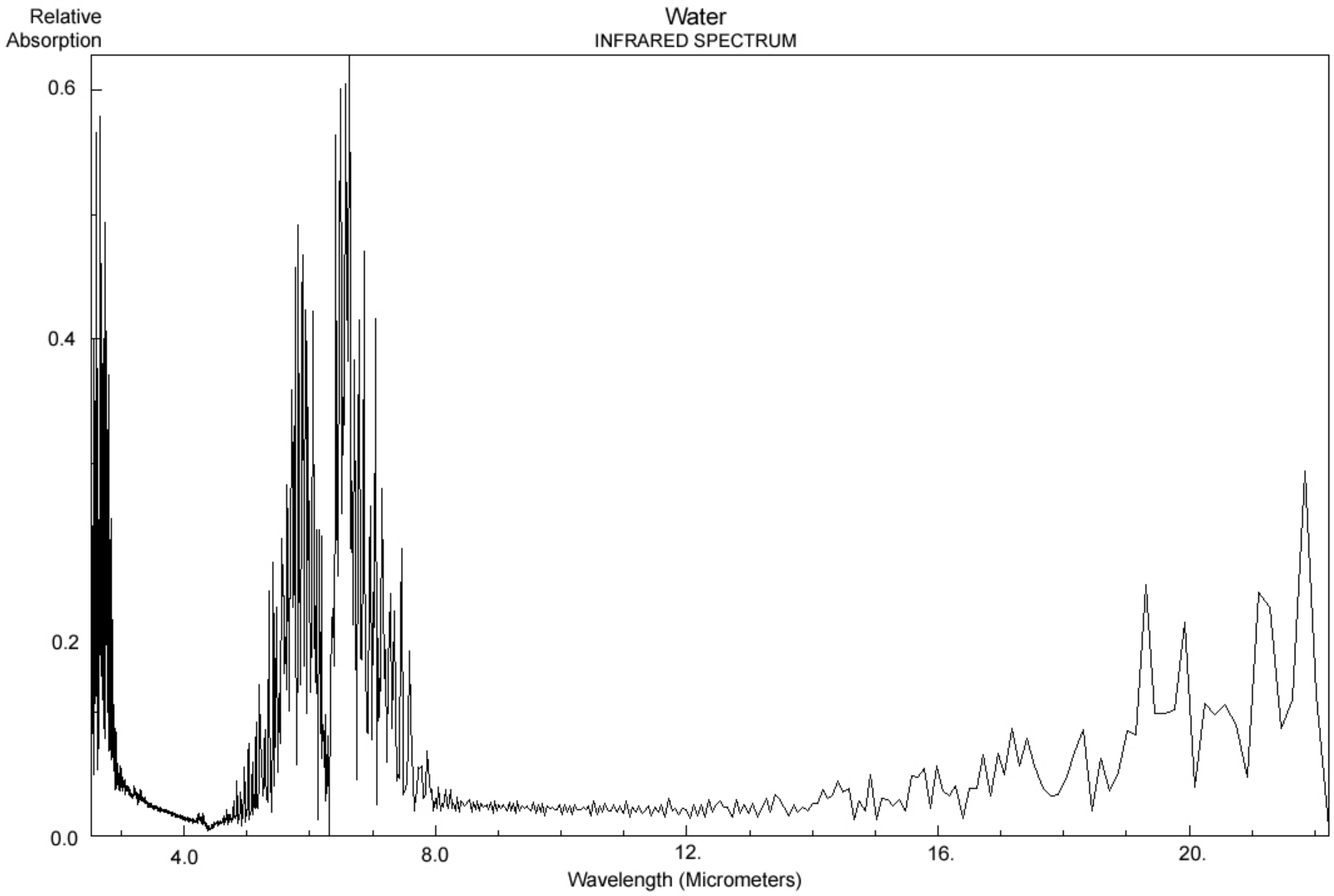
Relative Absorption
Water
INFRARED SPECTRUM
0.6
0.4
0.2
0.0
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)

Fig. 1

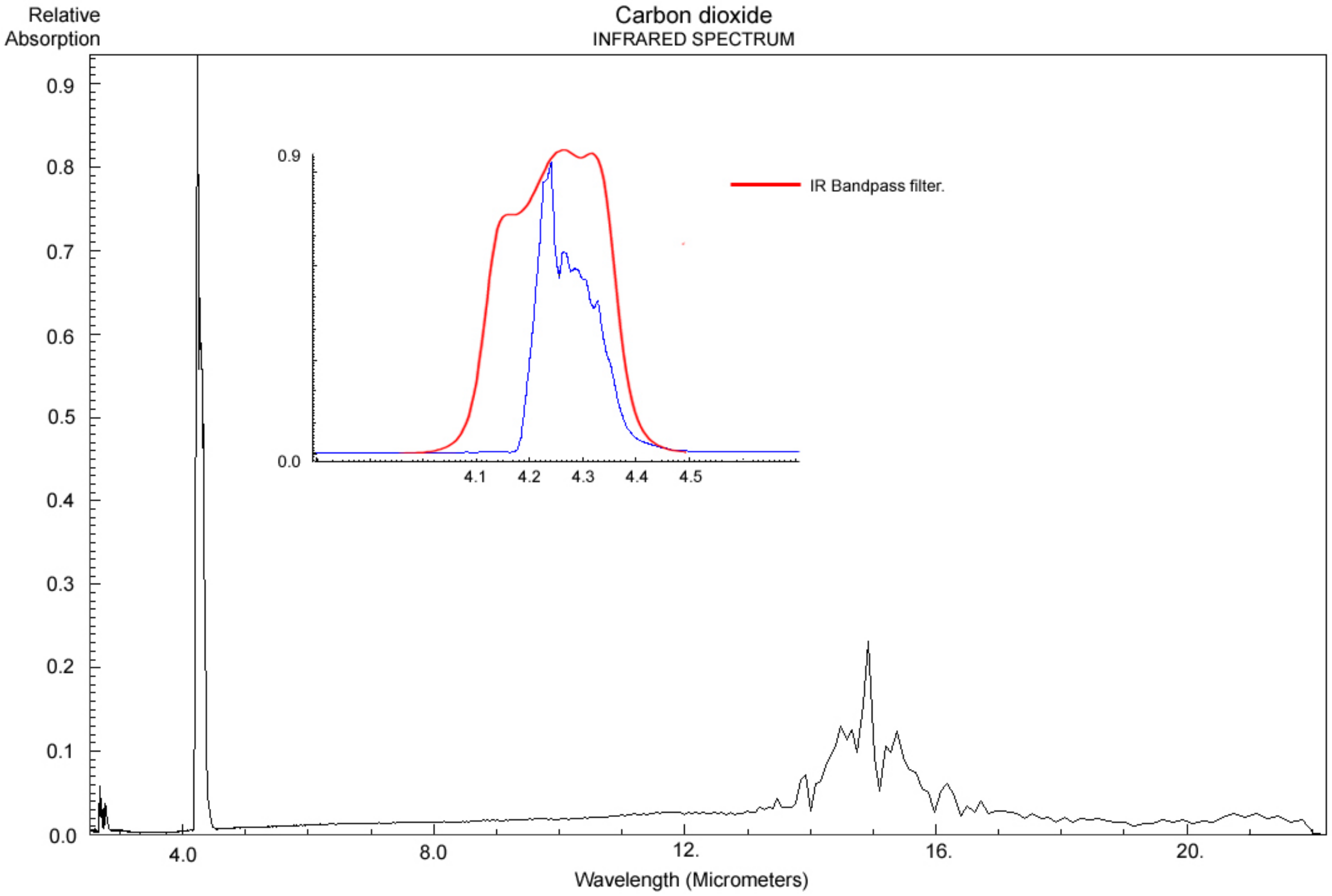
Relative Absorption
Carbon dioxide
INFRARED SPECTRUM
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.9
0.0
4.1
4.2
4.3
4.4
4.5
IR Bandpass filter.
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)

Fig. 2

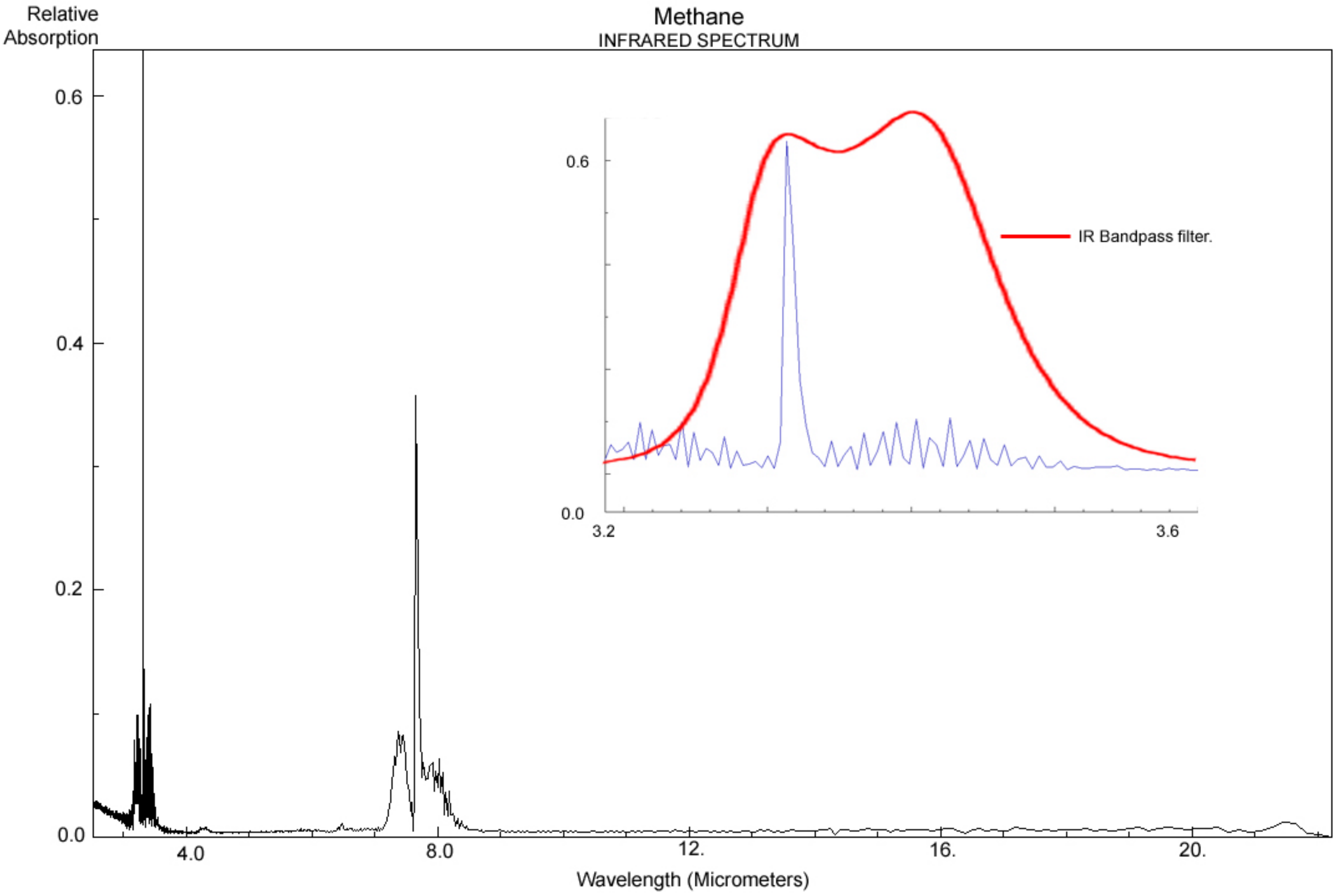
Relative Absorption
Methane
INFRARED SPECTRUM
0.6
0.4
0.2
0.0
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)
0.6
0.0
3.2
3.6
IR Bandpass filter.

Fig. 3

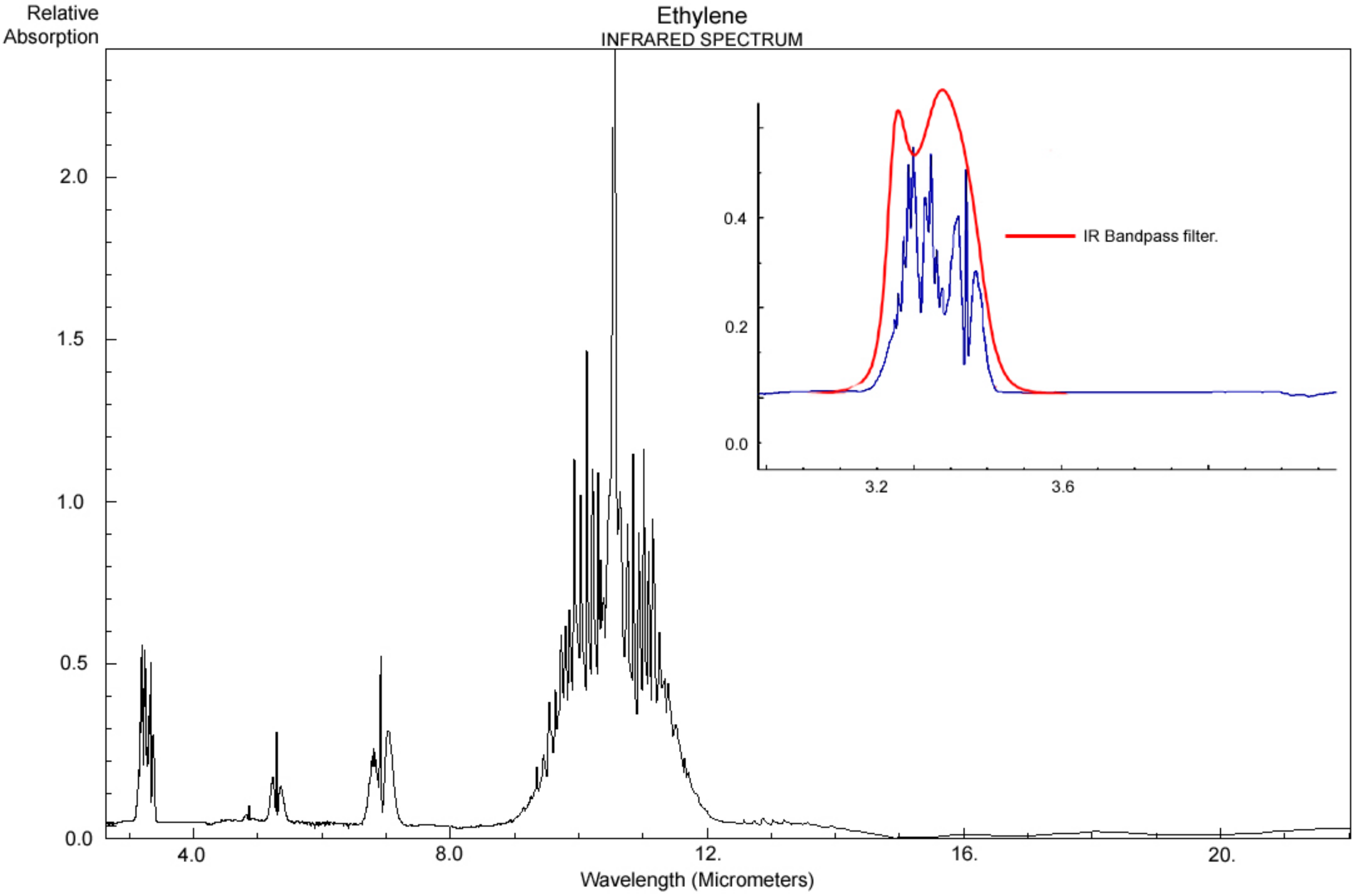
Relative Absorption
Ethylene
INFRARED SPECTRUM
2.0
1.5
1.0
0.5
0.0
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)
0.4
0.2
0.0
3.2
3.6
IR Bandpass filter.

Fig. 4

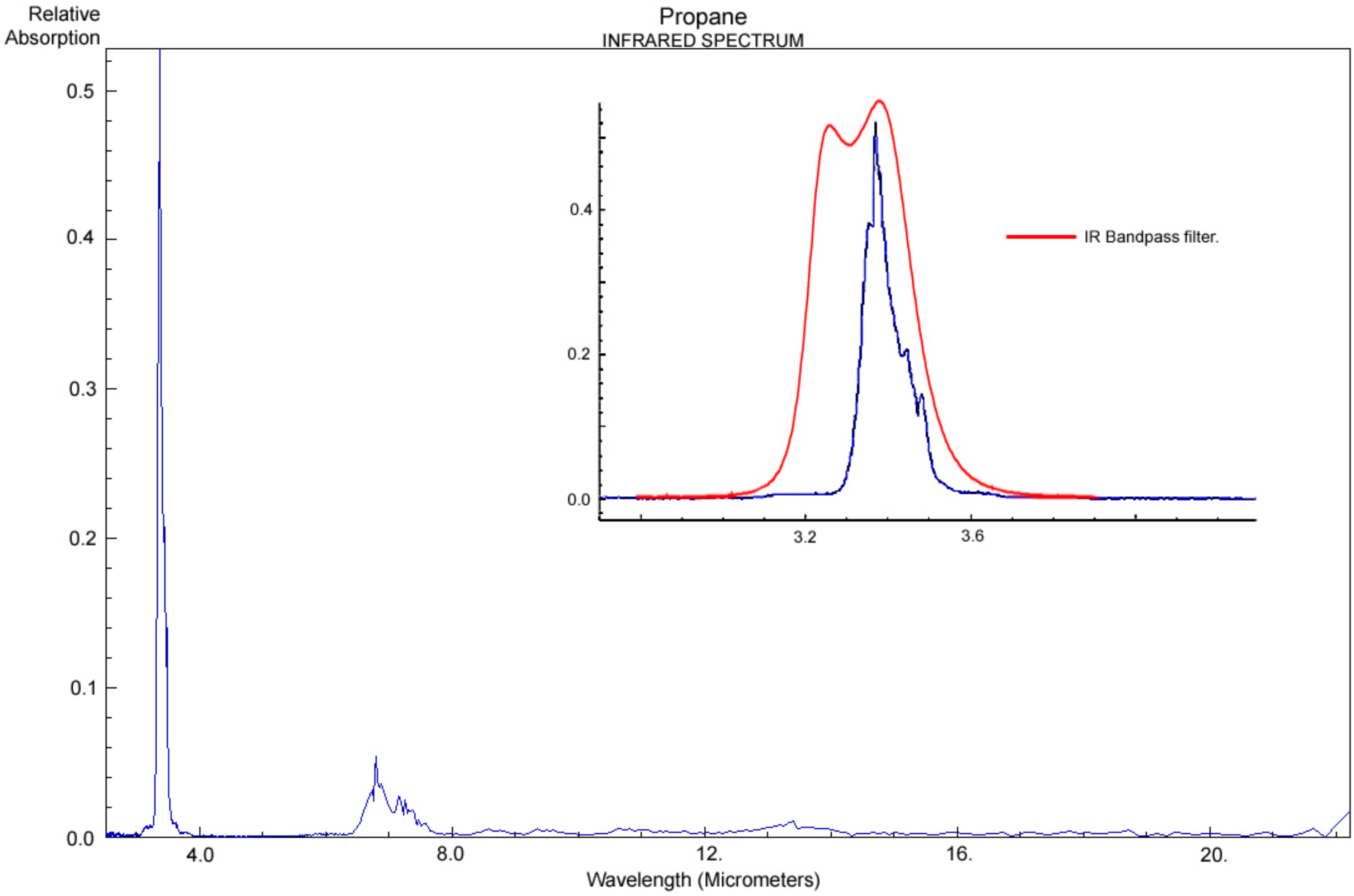
Relative Absorption
Propane
INFRARED SPECTRUM
0.5
0.4
0.3
0.2
0.1
0.0
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)
0.4
0.2
0.0
3.2
3.6
IR Bandpass filter.

Fig. 5

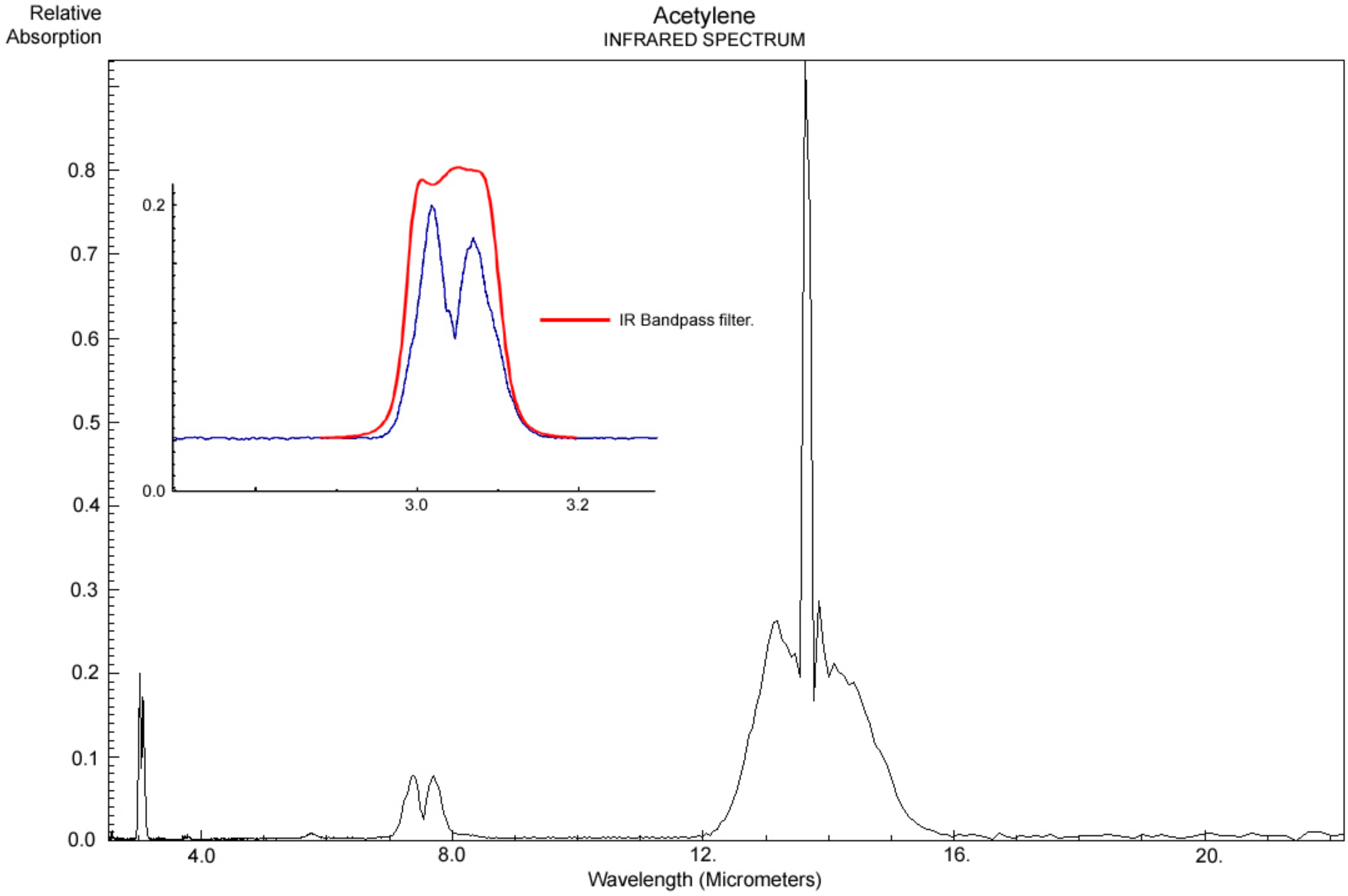
Relative Absorption
Acetylene
INFRARED SPECTRUM
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
4.0
8.0
12.
16.
20.
Wavelength (Micrometers)
0.2
0.0
3.0
3.2
IR Bandpass filter.

Fig. 6

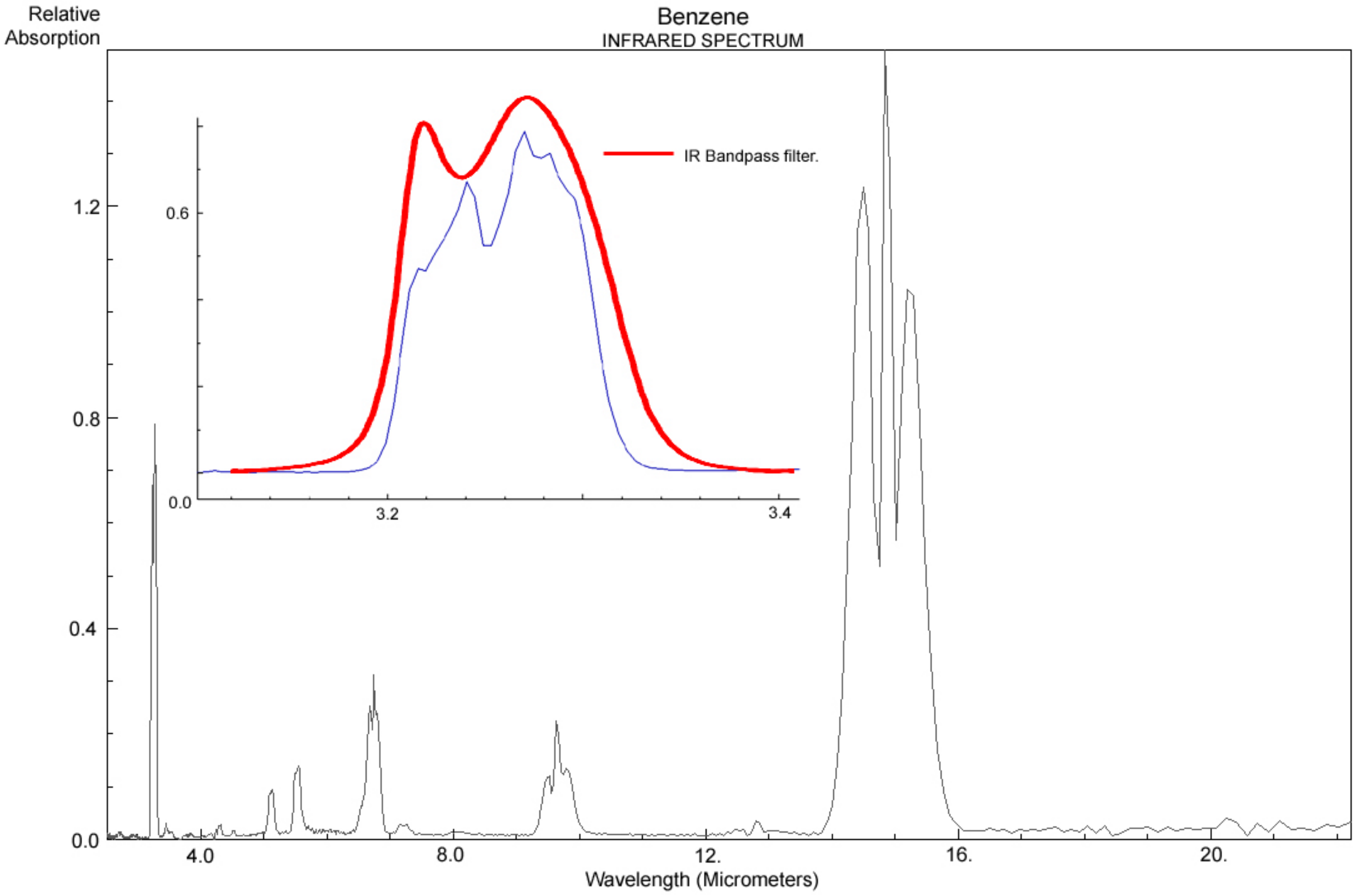

Fig. 7

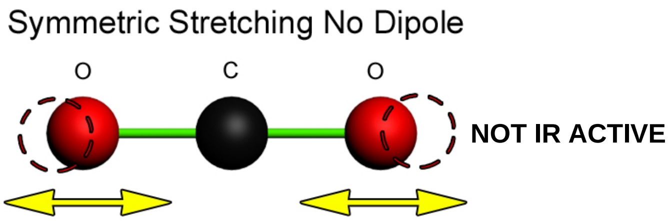

Fig. 8a

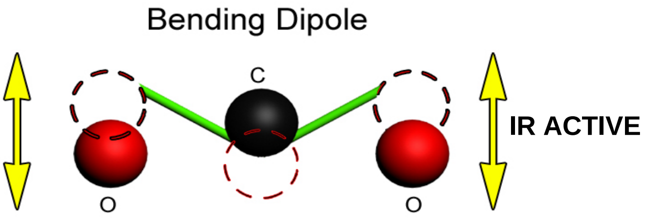

Fig. 8b

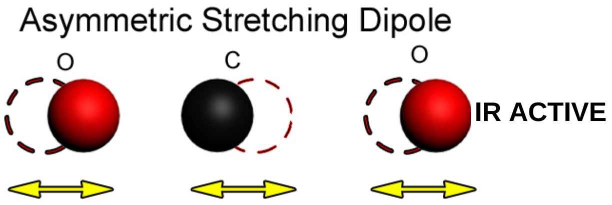

Fig. 8c

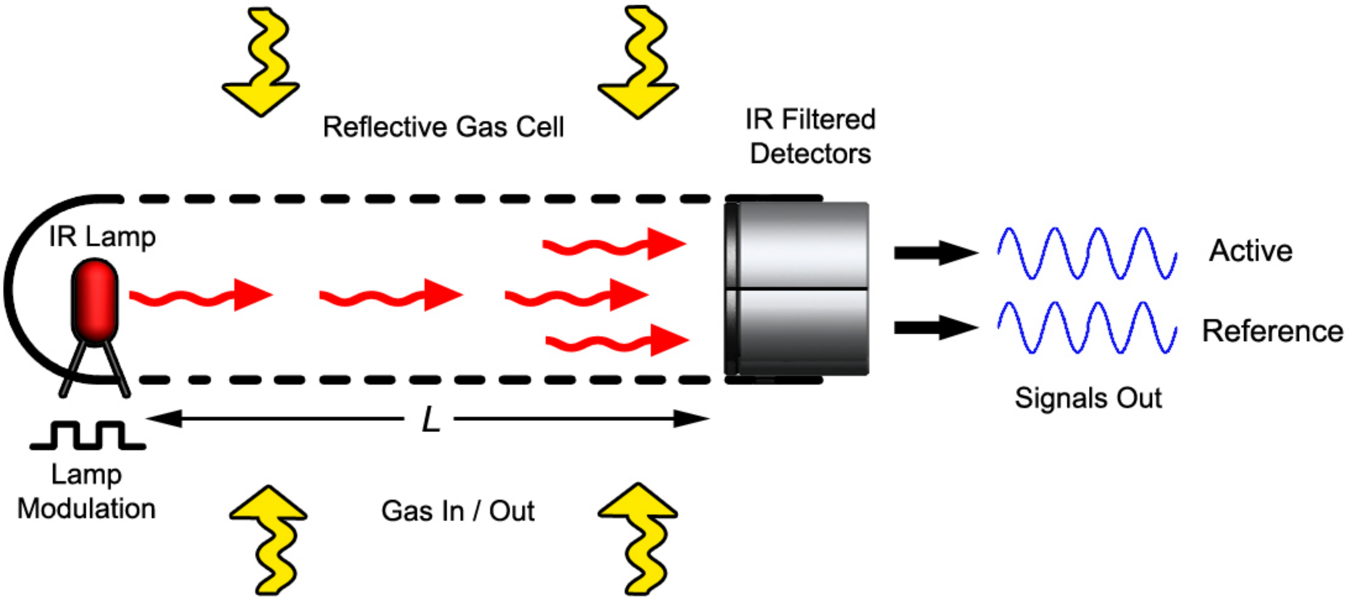

Fig. 9 NDIR Gas Sensor Schematic

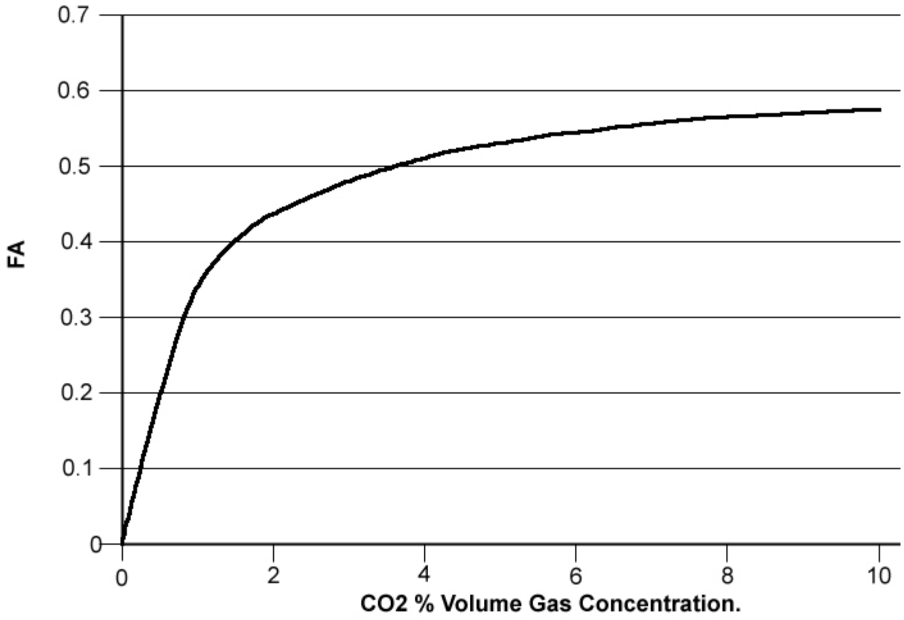

Fig. 10 Typical Fractional Absorbance