Theoretical model to predict the response of correlation spectroscopy gas detection systems

P. Chambers, E. A. Austin and J. P. Dakin.
Optoelectronics Research Centre,
University of Southampton, United Kingdom, SO17 1BJ.

Abstract

We present the first comprehensive model for the detection of a gas by absorption based correlation spectroscopy, and show the practically useful results obtained. Predictions of sensor response for a fibre-optic-coupled O_2 detection system have been made, based on gas absorption data from the HITRAN database. Fractional absorption-change values (modulation depth) were predicted, and system S/N values were derived, taking into account effects of fundamental photon noise limitations and thermal noise contributions. A new theoretical procedure for determining the optimum optical filter width and central wavelength for best modulation depth and best signal to noise (S/N) ratio is introduced. Using typical parameters associated with available optical components, practically achievable modulation depths, S/N ratios and O_2 detection limits have been derived.

1. Introduction

Absorption based correlation spectroscopy offers an attractive method to detect several gases of industrial importance. To-date no complete theoretical analysis of such a system has been presented and we now present such an analysis. As a case study, a correlation spectroscopy based O_2 sensing system was modelled, using published gas absorption data from the HITRAN database (http://www.hitran.com). Fractional changes in the detected response expected when gases are introduced into a correlation spectroscopy sensor system (we shall call this fractional change the modulation depth/index) were predicted and system signal to noise (S/N) values were derived, taking into account the effects of fundamental photon noise limitations and thermal noise contributions. We have shown that the model agrees well with experimental data which we have previously published.

2. Principle of Operation

There are several methods for detecting gases using correlation spectroscopy [1-13]. An attractive absorption based method is the correlation spectroscopy Complementary Source Modulation (CoSM) method [14-16]. This involves the alternate on/off switching of two light sources in anti-phase, passing light from one of these sources through a reference cell containing the target gas (or gases) of interest for detection, and then combining this now partially-absorbed light beam with a fraction of unaffected light from the other source, in a proportion such as to give no net intensity modulation over an appropriately optically filtered bandwidth. This combined beam is then used to probe for the target gas. As the beam component which has passed through the reference gas sample now has less available optical energy lying within the narrow spectral regions of the target gas spectral absorption lines, a net intensity modulation of the balanced combined beam will be re-established when it passes through a measurement cell containing the gas of interest. This induced intensity modulation is approximately proportional to the target gas concentration, as only differential absorption between the two beam components can contribute to a signal modulation. A fibre optic based schematic of an absorption based correlation spectroscopy gas sensing system is shown in figure 1. The input signal detector is used to ensure balanced light power and the output signal detector is used to evaluate any intensity modulation resulting from test gas in the measurement cell.

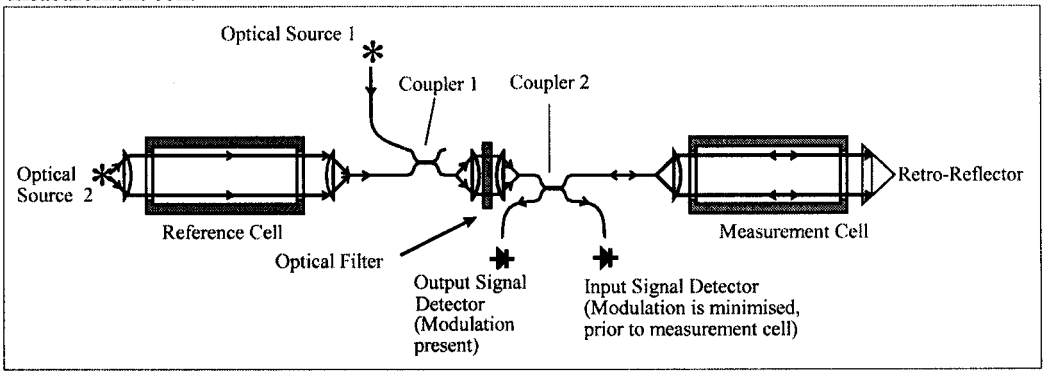

Figure 1: Schematic of a fibre optic based implementation of an absorption correlation spectroscopy system.

2. Modelled system parameters

It is important to model the correlation spectroscopy system, not only to predict performance, but also to make the very important selection of what type of optical filter (or what type of LED or super-luminescent optical fibre source in terms of optical spectral output) to use to achieve the best detection performance or best selectivity. We have defined and analysed the parameters that determine the system performance.

2.1 Modulation Depth

The first practically important system parameter that needs to be modelled is the modulation depth present at the output detector. This is effectively a measure of optical "contrast", and is defined as the peak to peak AC output signal variation arising when gas is introduced into the measurement cell, divided by the mean DC detected level.

Assuming that a spectrally-flat optical source is used and that the optical intensities at the reference detector are equalised, the Modulation Depth (MD) may be expressed as an optical intensity ratio. This is described in terms of the optical transmission of the reference and measurement gas cells, ($T_{Ref}(\lambda)$ and $T_{Meas}(\lambda)$, respectively) and the transmission spectrum of the optical filter ($F(\lambda)$):

$$MD = \frac{\int T_{Ref}(\lambda)T_{Meas}(\lambda)F(\lambda)d\lambda \int F(\lambda)d\lambda - \int T_{Ref}(\lambda)F(\lambda)d\lambda \int T_{Meas}(\lambda)F(\lambda)d\lambda}{\int T_{Ref}(\lambda)T_{Meas}(\lambda)F(\lambda)d\lambda \int F(\lambda)d\lambda + \int T_{Ref}(\lambda)F(\lambda)d\lambda \int T_{Meas}(\lambda)F(\lambda)d\lambda} \quad (1)$$

If desired, the source spectrum can also, of course, also be taken into account in equation 1, by using additional spectral functions as suitable product terms.

2.2 Other parameters that dictate system performance

To obtain maximum spectral contrast, the optical filter returning maximum modulation depth (equation 1) should be chosen, thereby reducing the sensitivity of the sensor system to environmental effects, such as dust in sensing cells or mechanical vibration. However, for good selectivity, and to improve the S/N ratio, it is also desirable to cover many gas absorption lines. A different choice of filter, to that required for maximum modulation depth, may therefore be required to obtain optimum S/N ratio, and to include sufficient gas lines.

3. Numerical Model Results

Below, optimal filters for modulation depth and S/N ratio are derived for an O_2 gas sensor operating at approximately 760nm.

3.1 Detection of oxygen gas (O_2) using 760nm absorption band.

Oxygen gas (O_2) exhibits an electronic based absorption band at approximately 760nm, the spectrum of which is shown in figure 2. Although this is just beyond the visible region, LED and tungsten optical sources and many commonly available passive optical components function well here. It is therefore relatively straightforward to implement optically based detection systems in this spectral region.

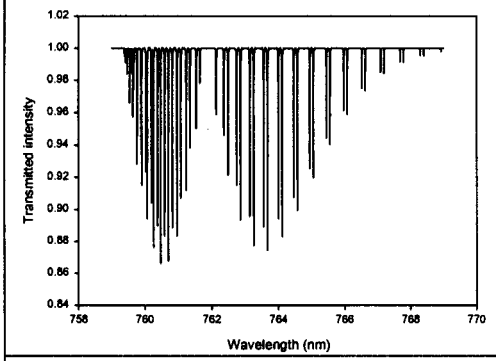

Figure 2: Spectral transmission of 100% O_2 gas, in the near IR region, over a 1m path at STP. (Source is HITRAN database)

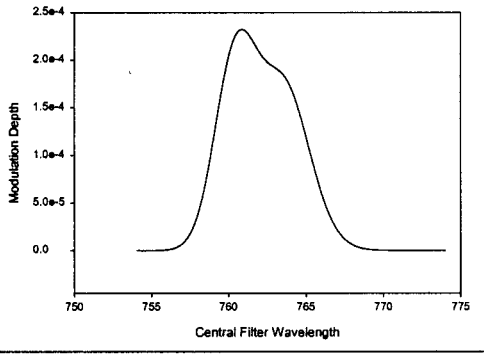

Figure 3: Theoretical variation of the modulation depth, as the centre wavelength of the Gaussian-shaped optical filter is changed.
Assuming reference and measurement cells contain 100% O_2 at STP and the Gaussian-shaped optical filter has a 3nm bandwidth.

3.2 Dependency of Modulation Depth on the central wavelength and bandwidth of the optical filter. Modelling the optical filter as having a Gaussian shaped transmission function, we have determined the dependency on the output signal modulation depth, on both its centre wavelength and its full width at half maximum bandwidth of the optical filter. Varying the centre wavelength first, the result shown in figure 3, shows that, with a 3nm Gaussian-shaped optical filter bandwidth, an optimum modulation depth (or optical contrast) is achieved at a filter centre wavelength of 760.9nm.

We then examined the effect of broadening the bandwidth of the Gaussian-shaped optical filter on the output signal modulation depth. To illustrate this, we performed calculations at two wavelengths, 760.9nm and 760.8nm, the first wavelength lying midway between two O_2 absorption lines, the second centred on a line. Under the same conditions, with the both cells again containing 100% O_2, figures 4(a) and 4(b) show the expected modulation depth at 760.9nm and 760.8nm, respectively, as the bandwidth of the Gaussian-shaped optical filter is increased from 0nm to 10nm. The modulation depth in figure 4(a) starts at zero, as the centre wavelength is between absorption lines, whereas that in figure 4(b) starts at a maximum as it is on a line. A further maximum in modulation depth is achieved in both plots at a Gaussian-shaped optical filter bandwidth of approximately 0.3nm. This is not a very practical choice for other reasons, however, and we will show later that choosing a significantly larger bandwidth, of around 3 nm, is more realistic when S/N considerations are included.

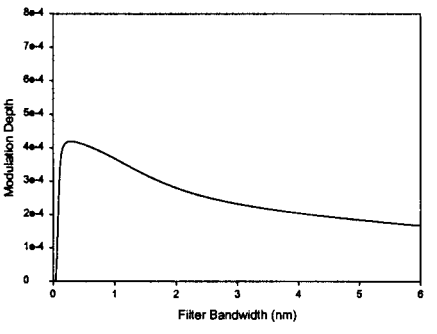

Figure 4(a): Modulation depth vs. bandwidth of a Gaussian-shaped optical filter centred at 760.9nm (off a spectral line)

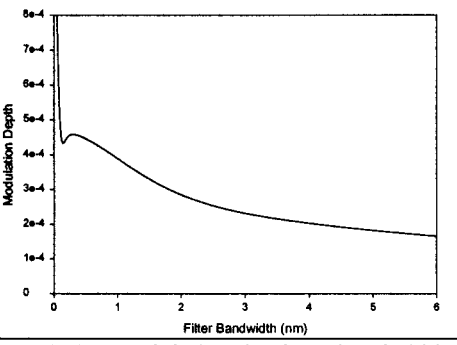

Figure 4(b): Modulation depth vs. bandwidth of a Gaussian-shaped optical filter centred at 760.8nm (on a spectral line)

Reference and measurement cells, containing 100% O_2, are of length 1m and at STP.

The dependency of the modulation depth on varying measurement cell O_2 concentration, when using a system with a 3nm bandwidth Gaussian-shaped optical filter, centred at 760.9nm, is shown on both linear and logarithmic scales in figures 5(a) and 5(b) respectively. These plots clearly show the almost linear relationship between modulation depth and a wide range of O_2 concentration in the measurement cell.

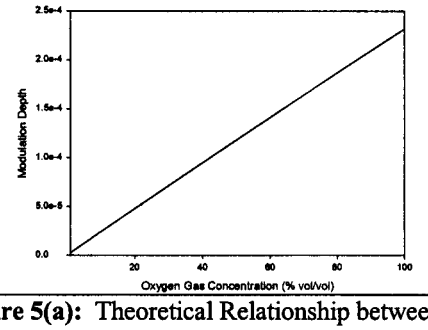

Figure 5(a): Theoretical Relationship between Modulation depth and O_2 concentration (vol/vol) in the measurement cell, plotted on a linear scale.

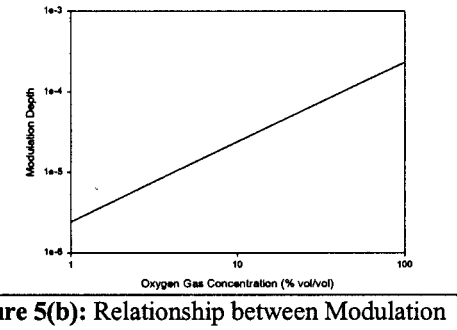

Figure 5(b): Relationship between Modulation depth and O_2 concentration (vol/vol) in the measurement cell, plotted on a logarithmic scale.

Reference and measurement cells are both of 1m length and reference cell contains 100% O_2 at STP. Gaussian-shaped optical filter has a bandwidth of 3nm and is centred at 760.9nm.

3.3 Gas Sensitivity Optimisation with respect to S/N Ratio.

Based on measurements from our earlier experimental results [16], we have assumed the received spectral intensity at the output detector is 10nW/nm. Our detection system used a silicon detector diode, followed by a FET based transimpedance amplifier, with a 10MΩ feedback resistor ($R_{Feedback}$).

The total noise contribution of the system was modelled by considering contributions of both photon and thermal noise on the output detector, given by equations 2 and 3 respectively:

$$I_{Photon\ noise} = \sqrt{2qI_{Sig}B} \quad (2) \qquad V_{Thermal\ noise} = \sqrt{4kTBR_{Feedback}} \quad (3)$$

where q is electronic charge, k is the Boltzmann constant, T is absolute temperature (modelled as 293°K), I_{sig} is the DC output current of the output detector and B is the detection bandwidth (modelled as 0.1Hz). Figure 6 shows the voltage noise at the output detector (left axis, solid line) and the increase in the AC amplitude of the measurement signal (right axis, dashed line) as the Gaussian-shaped optical filter bandwidth is increased.

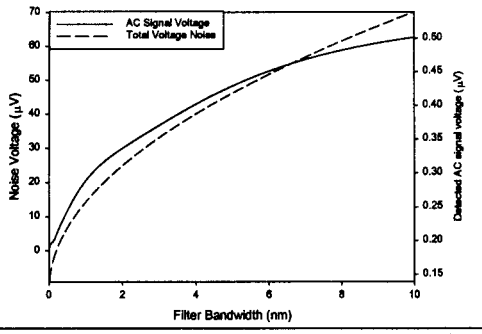

Figure 6: Graph of expected AC signal modulation (dashed line, right Y axis) and calculated noise voltage (solid line, left Y axis), as bandwidth of Gaussian-shaped optical filter is changed.

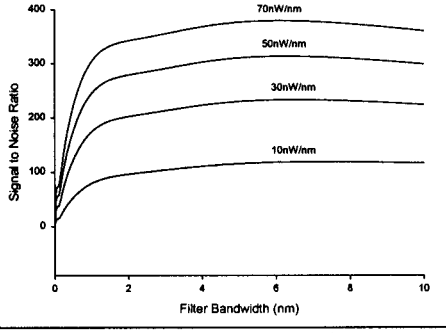

Figure 7: Predicted variation in S/N ratio as the bandwidth of the Gaussian-shaped optical filter (centred at 760.9nm) is changed. This is shown for four detected output optical power levels.

Reference and measurement gas cells are of 1m length and contain 100% O_2 at STP.

Figure 7 shows that best S/N ratio is attained with a Gaussian-shaped optical filter bandwidth of approximately 7nm, whereas best contrast was achieved with a bandwidth of approximately 0.3nm. We consider that a 3nm bandwidth offers a reasonable compromise between these two extremes. Figure 7 also shows that increasing the signal light intensity level has a relatively small effect on the bandwidth of the Gaussian-shaped optical filter needed to obtain an optimised S/N ratio.

Due to the near-linear relationship between the concentration of O_2 in the measurement cell and the modulation depth, the inverse of the S/N values are also representative of the minimum detectable concentration of O_2 in the measurement cell, i.e. the concentration at which SNR=1.

3.4 Cross sensitivity

We examined the cross sensitivity of a correlation spectroscopy based system to contaminant gases. The correlation spectroscopy method, as described by equation 1, has the property that the cross sensitivity to a contaminant gas is small, even when it has non-coincident optical absorption lines in the same spectral region as that of the target gas. We illustrate this by modelling the response of an O_2 detection system to realistic concentrations of the OH radical, characteristic of water vapour, which is one of the few likely gaseous contaminants with absorption around 760nm.

Figure 9 shows a plot of the theoretical improvement, in rejection factor, that an absorption based correlation spectroscopy system provides, compared to a simple broadband absorption detection system. Realistic concentrations (0%-4%(vol/vol)) of contaminant OH and a range of Gaussian-shaped optical filter central wavelengths are considered. This shows that a correlation spectroscopy system is approximately 200 times less sensitive to the OH radical than a simple broadband absorption based sensing system would be.

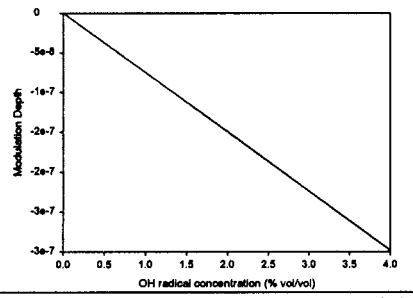

Figure 8: Near-linear dependence of Modulation Depth on concentration of gaseous OH contamination in measurement cell (Assumes Gaussian-shaped optical filter, of 3 nm bandwidth, centred at 760.9nm).

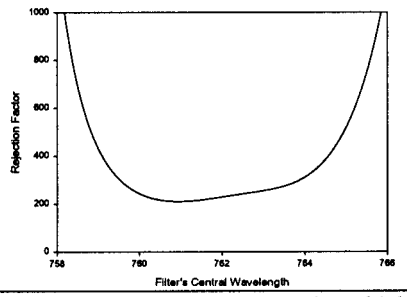

Figure 9: Rejection factor, or ratio by which an absorption correlation spectroscopy technique offers improved selectivity when compared to a simple optical absorption method (assumes Gaussian-shaped optical filter of 3nm bandwidth)

The graphs above assume a correlation spectroscopy system based on 1 m long reference cell, containing 100% O_2, and the measurement cell containing realistic concentrations of contaminant OH at STP.

3.5 Comparison with experimental results

We demonstrated earlier the experimental operation of an O_2 absorption based correlation spectroscopy system [16]. There, we used a Gaussian-shaped optical filter, centred at 762.6nm, with a bandwidth of 3nm, and a 1m reference cell containing 100% O_2 and a 0.8m measurement gas cell, containing air (21% O_2) at STP. We also considered a measurement cell of 1.6m equivalent length, when a retro-reflector arrangement was used. By inserting the relevant data into equation 1, we compared our new theoretical results with the experimental results that were previously obtained.

Theoretical comparison with experimentally derived predictions of modulation depth.			
Reference Cell pathlength	Measurement Cell pathlength	Experimental	Theoretical
1m	0.8m	2.8x10-5	3.2x10-5
1m	1.6m	5.6x10-5	6.4x10-5
Temperature and Pressure = STP	Reference cell O_2 concentration = 100%		
	Measurement cell O_2 concentration = 21% (vol/vol)(Air)		

Table 1: Theoretical comparison with experimentally derived predictions of modulation depth.

The experimentally obtained detection limit of less than 1% (vol/vol) O_2 concentration, in the early work, compares favourably with a theoretical derived predicted value of 0.6% (vol/vol) (obtained from our S/N analysis above).

4. Conclusions

We have reported new theoretically modelled results for gas detection using the CoSM scheme for absorption based correlation spectroscopy. This includes simulated responses of signal modulation depth, predictions of the S/N ratio that may be achieved, an analysis of the expected selectivity in the presence of a contaminant gas and finally a comparison of our theoretical predictions with previously published experimental data. In this work we have developed a model that allows us to determine which light sources, optical filters and detectors would give optimal detection of gases using absorption based correlation spectroscopy.

This work has shown that, as expected, the modulation depth response of an absorption based correlation spectroscopy system is strongly dependant of the type of optical filter chosen. The optimum bandwidth and centre wavelength of a Gaussian filter required to maximise the modulation depth in our O_2 sensing system was 0.3nm at 760.9nm. We have shown that, when other key aspects, such as achieving a good S/N ratio, are taken into account it may be better to use an optical filter of somewhat higher bandwidth, which will also improve selectivity by including more gas lines. For our O_2 sensing system, the best optical filter bandwidth for maximum S/N was found to be 7nm. Fortunately, the modulation depth, or measurement contrast, does not drop very rapidly beyond the peak at 0.3nm, so, choosing wider filter bandwidths to improve selectivity and S/N should not lead to a significant reduction in modulation depth (or measurement contrast). We intend to present results for an updated system as a result of these findings in the near future.

5. Acknowledgements

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