Theoretical analysis of a CO_2 gas detection system using correlation spectroscopy

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ABSTRACT

We present a comprehensive model of a CO_2 correlation spectroscopy based gas sensor. Predictions of the sensor response for typical fibre optic-coupled systems are made, taking into account effects of noise in detected signals.

1. INTRODUCTION

Absorption based correlation spectroscopy offers a method to selectively detect gases of industrial importance. We now present a complete theoretical analysis of such a system for the measurement of CO_2 (carbon dioxide) gas. The model has been used to predict fractional changes in the detected response (modulation index) expected when gases are introduced into the sensor. The system signal-to-noise ratio (SNR) has been derived, taking into account the effects of fundamental photon noise limitations and thermal noise contributions. The expected variation in the detected response over the normal variation of atmospheric temperature and pressure is also shown. The HITRAN database (http://www.hitran.com) was used to provide all gas transmission spectra.

2. PRINCIPLE OF OPERATION

There are several methods for detecting gases using correlation spectroscopy.[1] An attractive absorption based method is the correlation spectroscopy Complementary Source Modulation (CoSM) method.[2] 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. The 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 region of the target gas 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 reference signal detector is used to ensure balanced light power and the measurement signal detector is used to evaluate any intensity modulation resulting from test gas in the measurement cell.

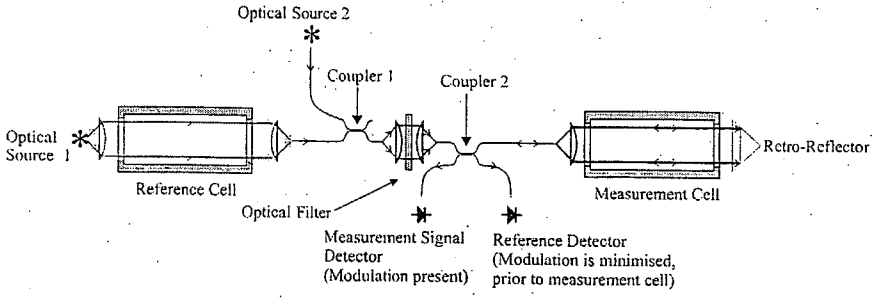

Figure 1. Schematic of a fibre optic based implementation of an absorption based correlation spectroscopy system.

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3. SYSTEM MODEL

It is important to model such a correlation spectroscopy system, to predict performance, and to aid the very important choice of optical filter (or choose the best LED or super-luminescent optical fibre source to give the optimal spectral output), in order to achieve the best detection performance or best selectivity. The length of the cells and the pressure of gas (or gas concentration) are also important parameters (although all results here are based on use of 1 m long cells).

The first practically important system parameter that should be modelled is the modulation index of the detected optical signal, as seen at the measurement detector, when target gas is present in the measurement cell. This fractional intensity change in the optical signal at this detector is effectively a measure of the optical "contrast" of the system. A small fractional change (low contrast) would give a high susceptibility to undesirable environmental effects, such as dust particles passing through the cells, mechanical vibration or modal noise arising from selective mode coupling in multimode fibres. It also means the optoelectronic feedback control scheme has to be particularly well balanced to avoid systematic errors. A high modulation index is therefore desirable, even though it is not the fundamental signal to noise limitation.

The modulation index is related to the transmission spectra of the gas-filled reference cell, $T_{Ref}(\lambda)$, the measurement cell, with its unknown gas composition, $T_{Meas}(\lambda)$, and the optical filter, $F(\lambda)$, all shown in equation 1. If required, the source spectra can also be taken into account, by using additional spectral functions (although this will usually have little spectral variation over the bandwidth of the gas band):

$$m = 2\left(\frac{\int F(\lambda)T_{Ref}(\lambda)T_{Meas}(\lambda)d\lambda \int F(\lambda)d\lambda - \int F(\lambda)T_{Ref}(\lambda)d\lambda \int F(\lambda)T_{Meas}(\lambda)d\lambda}{\int F(\lambda)T_{Ref}(\lambda)T_{Meas}(\lambda)d\lambda \int F(\lambda)d\lambda + \int F(\lambda)T_{Ref}(\lambda)d\lambda \int F(\lambda)T_{Meas}(\lambda)d\lambda}\right) \quad (1)$$

To reduce the sensitivity to environmental effects, the above modulation index should be maximised, but for good selectivity and to improve the fundamental SNR it is normally desirable to use a broader filter in order to cover more gas absorption lines. The effect of system parameters on these quantities is calculated below.

4. NUMERICAL RESULTS

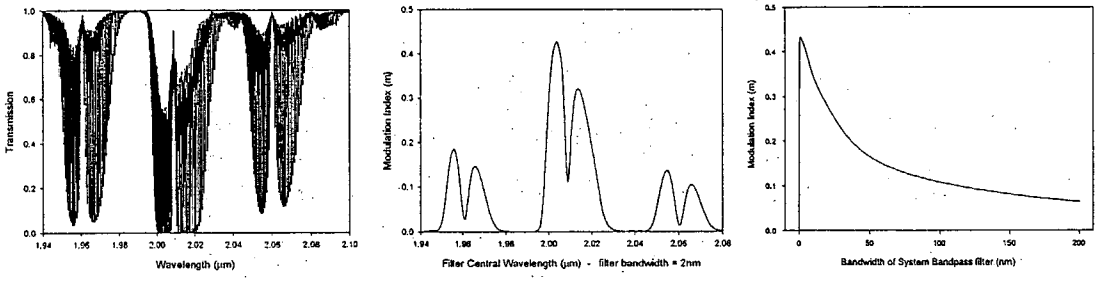
In this section, after showing the transmission spectrum of CO_2 gas, we show results from our model. The modulation index and SNR in measurements are shown. The susceptibility of the system to drifts in temperature and pressure will be shown in the poster presentation.

4.1. Transmission of CO_2 gas

CO_2 exhibits a strong rotational-vibrational $3v_3$ based absorption band at approximately 2.0 μm, the spectrum of which is shown in figure 2(a). Many commonly available optical sources and passive optical components function well in this wavelength range so it is relatively straightforward to implement optical systems in this spectral region.

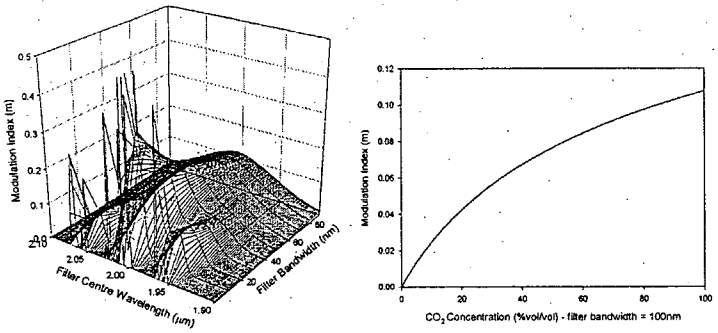
4.2. Received modulation index (optical 'contrast')

We initially calculated the effect of varying the central wavelength of a narrow-band Gaussian shaped optical filter (2 nm Full Width at Half Maximum -FWHM- bandwidth) on the modulation index, see figure 2(b). This shows that a clear peak in modulation index is achieved at an optical filter centre wavelength of 2.004μm, where CO_2 has a closely-spaced set of absorption lines. The optimum filter bandwidth for operating at this peak central wavelength was determined by plotting the modulation index as a function of filter bandwidth, as shown in figure 2(b). This shows the peak in modulation index actually occurs when using as narrow a filter bandwidth as possible and centering it on a single strong absorption line. However, it will be shown that such a narrow filter is not a practical choice either for good SNR or for good selectivity. Poor stability can also result, despite this high modulation index, as the narrow linewidth can give severe interference effects, particularly high modal noise due to selective mode coupling in multimode fibres. As this peak in modulation index response corresponds to an unrealistically narrow optical system filter, we searched for other peaks using wider bandwidth filters. Figure 3(a) is a 3D plot, showing the modulation index as a function of optical filter width and centre wavelength.



(a) (b) (c)

Figure 2. (a) Transmission spectrum of CO_2 gas over a 1 m path length at 20 °C and 1 Atm (transmission data was obtained from the HITRAN database). (b) Modulation index as a function of selection filter center wavelength, assuming reference and measurement cells contain 100% CO_2 at 1 Atm and 20 °C and the Gaussian-shaped selection filter has a 2 nm FWHM bandwidth. (c) Modulation index vs. filter bandwidth assuming reference and measurement cells, containing 100% CO_2 at 1 Atm and 20 °C, of length 1 m at 1 atm and 20 °C, and selection filter center wavelength of 2.004μm.



(a) (b)

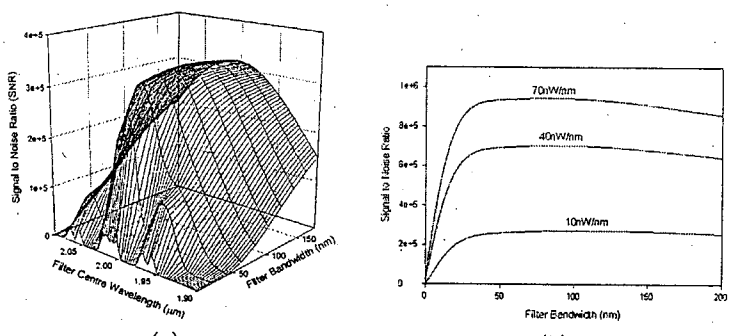
Figure 3. (a) Modulation index as a function the centre wavelength and bandwidth of the optical filter The broad range of strong absorption lines results in a very complex modulation index response. (b) Modulation index as a function of CO_2 concentration (%vol/vol) in the measurement cell, the optical filter was at a center wavelength of 2.004μm and a bandwidth of 100 nm. Conditions are as per previous graphs.

Optical filters with centre wavelengths between 1.90 μm and 2.1 μm, and bandwidths between 1 nm and 200 nm were considered. As can be seen, the modulation index behaviour is highly complex, with several other narrow bandwidth maxima in response. The very narrow bandwidth (2 nm) peaks are unsuitable, as will be shown, and there is no further clear peak. To optimize the system, it was therefore necessary to investigate the other system parameters, such as SNR in measurements. The response to varying CO_2 concentration is now considered. Figure 3(b) shows the dependency of modulation index on measurement gas cell concentration. This shows that, due to the strong absorption of the gas in this band, there is a substantial non-linearity in the modulation index response at higher CO_2 gas concentrations in the measurement cell. An optical filter bandwidth of 100 nm was assumed. As will shown later, this is a realistic predicted value.

4.3. Influence of selection filter on signal-to-nose ratio

Our model was used to predict system SNR performance, by predicting noise in measurements arising from fundamental photon noise and from thermal noise in the optical receiver circuit. We assumed a spectral intensity at the output detector of 10 nW nm^{-1}. A PIN detector of 0.5 A W^{-1} responsivity, followed by a transimpedence amplifier with a 10MΩ feedback resistor ($R_{Feedback}$) was assumed.

Based on these assumptions, the total noise in measurements at the output detector was modelled in terms



(a) (b)

Figure 4. (a) SNR in measurements as a function of selection filter choice. It was assumed that 10 nW nm^{-1} spectral power would be received at the detector if the measurement gas cell had no absorption. (b) SNR at 3 different received optical power levels

of photon (2) and thermal (3) noise contributions.

$$I_{ShotNoise} = \sqrt[2]{2qI_{Sig}B} \quad (2)$$

$$I_{ThermalNoise} = \sqrt[2]{\frac{4kTB}{R_{Feedback}}} \quad (3)$$

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 measurement detector and B, the detection bandwidth, is assumed to be 0.1 Hz. Figure 4(b) plots the SNR expected as a function of optical filter bandwidth and centre wavelength for a variety of received optical intensities. The SNR ratio is not very dependent on filter centre wavelength, but is strongly related to the filter bandwidth. Optimum SNR ratio is attained with a filter width of approximately 100 nm, i.e. much wider than the very narrow value required to maximize modulation index. Figure 4(a) shows SNR versus filter bandwidth and centre wavelength.

5. CONCLUSIONS

We have used a theoretical model for gas detection systems using the CoSM scheme for absorption based correlation spectroscopy to predict the response and performance of a CO_2 sensor. Component characteristics for best signal-to-noise and selectivity to CO_2 were predicted. This work has shown that, as expected, the modulation index response of an absorption based correlation spectroscopy system is strongly dependant on the type of system optical filter chosen. For optimum modulation index (measurement contrast), an optical filter having centre wavelength 2.004 μm and a very narrow bandwidth would be chosen, this would select too few lines to give the selectivity and other advantages of correlation spectroscopy. We have shown that, when other key aspects, such as achieving a good SNR, are taken into account it may be better to use an optical filter of somewhat higher bandwidth. The best SNR is achieved with a filter of width 100 nm. Fortunately, following an initial peak, the modulation index, or measurement contrast, does not drop very rapidly beyond bandwidths of around 100nm so; choosing wider filter bandwidths to improve selectivity and SNR should not lead to too great a penalty in modulation index. The sensor is expected to be highly selective.

REFERENCES

1. R. Goody, "Cross-correlating spectrometer," *Journal of the Optical Society of America* **58**(7), pp. 900–908, 1968.
2. J. P. Dakin, M. J. Gunning, P. Chambers, and Z. J.Xin, "Detection of gases by correlation spectroscopy," *Sens. & actuators B,: Chem* **90**, pp. 124–131, 2003.