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Non-dispersive infra-red (NDIR) measurement of carbon dioxide at $4.2 \, \mu m$ in a compact and optically efficient sensor



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ABSTRACT

Non-dispersive infra-red (NDIR) gas detection has enjoyed widespread uptake as a result of development of devices in the standard miniature format for gas sensors, consisting of a cylinder with external dimensions of 20 mm diameter \times 16.5 mm height. We present a new design for such a sensor, making use of low-cost injection moulding technology. The design pays particular attention to the problem of maintaining a high optical throughput while providing an acceptable optical pathlength for gas detection. A detailed analysis of the design is presented, with the results of optical raytracing, showing a raytrace estimate for 4% of the total emitted radiation reaching each of two separated detector elements and a pathlength of 32 mm. Finally, we show experimental results obtained with as-manufactured devices, with a short-term limit of detection for carbon dioxide (CO₂) estimated at 1 ppm or a noise equivalent absorption (NEA) of 3×10^{-5} AU.

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1. Introduction

Non-dispersive infrared (NDIR) gas sensing is one of the most widely used optical gas detection techniques, and there is a wide range of cell designs in commercial manufacture [1]. For some gases, notably carbon dioxide (CO₂), alternative (non-optical) technologies are unsuitable and therefore CO₂ detection in low-cost, volume applications often incorporates an NDIR sensor. These applications include heating, ventilation and air conditioning (HVAC) control [2], industrial safety especially in the brewing industry (CO₂ is an asphyxiant), process control and capnography (the measurement of time-resolved CO₂ concentration in exhaled breath) for patient monitoring for example during anaesthesia [1].

There are few alternative sensor technologies capable of detecting CO_2 at ppm concentrations. Devices have been developed based on the electrochemical principle [1] and research is also underway on metal oxide semiconductors for CO_2 . However, both techniques are known to cross-respond to other gas species, including water vapour, whereas NDIR sensors for CO_2 are considered to be specific to that species alone [1]. Furthermore the development of metal oxide sensors capable of detecting CO_2 below 2000 ppm is "the biggest challenge" according to a recent review [3].

Over the last decade, the commercial market has become populated with small footprint gas sensors based on the NDIR principle

[4]. The dimensions of these sensors (a cylinder $20\,\mathrm{mm}$ diameter \times $16.5\,\mathrm{mm}$ high) follow a default standard for the gas sensor industry that we will refer to throughout this paper as the standard miniature format. Thus, equipment manufacturers need not alter the dimensions of their housings when switching to NDIR sensors.

These sensors are low cost, having few components (typically a simple microbulb light source, gold coated reflective light path and detector) [5]. The microbulbs used in conventional NDIR sensors have two main advantages; their spectral emission is relatively high (2 mW per steradian in a FWHM bandwidth of 0.17 µm at $4.2 \,\mu\text{m}$, for one example [6]) and the cost is low (\$1-2 [6]). A key to the miniaturisation of this technology has been the integration of multiple detectors and filters into a small single package, typically a 9 mm diameter TO-5 can [7]. Commercially available sensor designs in the standard miniature format include a dual ellipsoid/reflector/ellipsoid arrangement [8], a pathlength arranged in the form of a spiral around the bulb/detector [9], and a mini integrating sphere with a rough internal surface, in which the light bounces around the internal cavity at random until it is absorbed by the sidewalls, the gas sample, or the detector [9]. However, detailed optical analysis of these compact designs has been limited, as is the use of injection moulding technology, which offers a potentially wider range of design options. A recent design with an LED source and photodiode integrated on an electronic chassis uses injection moulded reflective optics [10], with the simplest optical design having both emitter and detector as close as possible to the centre of a hemisphere. However its use of an LED is restrictive as such devices are currently significantly more costly than microbulbs.

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Research in this area has concentrated on the following requirements; (i) the need for compact cells, (ii) maximising the pathlength to optimise sensitivity, and (iii) the need to maximise the proportion of light coupled through the cell to the detector, in order to overcome the detector noise limit.

Fonollosa et al. have developed a high numerical aperture (NA) Fresnel lens formed in silicon (transmissive in the mid IR) to make a light-efficient and ultra-compact dual band detector [11]. The detector module has been integrated into a system for measuring ethylene in agricultural storage, with a 30 ppm detection limit [12]. Further miniaturisation may also result from work to integrate detectors and filters on a single base substrate [13].

The light collection efficiency of an optical system may be defined using the 3D étendue, equal to the product of the light beam's area and its solid angle. The proportion of light passed from one element of the system to the next is proportional to the étendue, and the overall throughput (T) can be defined as [14]:

$$T = A\Omega\rho \tag{1}$$

At the limiting aperture, A is the area of the aperture, Ω is the solid angle and ρ accounts for additional losses in the system, for example due to the reflectivity of mirrors being less than 100%. To design a high efficiency cell, one must maintain a high étendue throughout the system, which demands the use of large apertures and/or high NA optics throughout. Constraints on the cell volume will therefore impact on the optical pathlength, or optical efficiency, or both. It is for this reason that the design of a compact, optically efficient cell presents a challenge. Typically within a 20 mm diameter \times 16.5 mm high sensor (external dimensions) are the 9 mm diameter detector and 3.2 mm diameter \times 6.4 mm long cylindrical microbulb, which leaves little room for manoeuvre when designing the optical path.

Various groups have reported studies of novel gas cell designs using a ray tracing approach. Mayrwöger et al. have used the Zemax software package to evaluate 3 different cell designs including a hollow, internally reflective tube (25 mm long \times 3 mm diameter), an internally reflective ellipsoid (principal axes 55 mm and 20 mm) and a spiral design within a cylinder of dimensions 30 mm diameter \times 10 mm height [15]. Each design incorporated a standard microbulb and a single element detector within a 9 mm diameter TO-5 can. For the latter two designs, mean optical pathlengths of 140 mm and 980 mm were reported from the ray trace simulations. The first (tube) design was used in combination with a bolometer detector to measure CO₂ with a limit of detection of around 150 ppm [16].

Sieber et al. have also reported a method for optimising a ray traced design for a chamber containing a curved surface that focused light from source to detector [17]. In particular, they showed the effect of positioning of the source on the irradiance distribution in the chamber, and reported how the overall gas detection performance was to be modelled. Their chamber was 42 mm long, with a mean pathlength of 60 mm. An optical cell with similar dimensions and elliptical reflectors has also been developed, and used by Hök et al. in the detection of breath ethanol [18]. Multiple reflections provided a pathlength of 210 mm within a package of approximately $40 \text{ mm} \times 40 \text{ mm} \times 14 \text{ mm}$.

Viola has reported on the development of a multipass NDIR cell with an acceptance NA of 0.22 and source/detector areas of 5 mm \times 5 mm each [14]. Collection efficiency was 3.7 sr mm² and overall throughput (taking into account multiple reflections from gold surfaces with 95% reflectivity) was estimated to be 2.2 sr mm². The overall physical length of the gas cell was >120 mm, and multiple passes between two off-axis parabolic mirrors and two retroreflectors yielded an optical pathlength of 940 mm. Optical performance has been validated and the device has been used to detect ammonia at 10.5 μ m [19].

Despite this activity, to date none of this reported work has been applied to sensors as small as the standard miniature format. In this paper, we report on the modelling and realisation of a novel gas cell design that fits within these external dimensions of a 20 mm diameter \times 16.5 mm height cylinder, translating to internal dimensions for the optics of 17.5 mm diameter and 10.5 mm height.

2. Principle of operation

For monochromatic light, the Beer-Lambert law gives the level of light *I* transmitted through an absorbing medium such as a gas [20],

$$I = I_0 \exp(-\alpha \ell) \tag{2}$$

where I is the light transmitted through the gas cell, I_0 is the light incident on the gas cell, α is the absorption coefficient of the sample (units of cm⁻¹) and ℓ is the cell's optical pathlength (units of cm). The absorption coefficient α is the product of the gas concentration (for example the partial pressure in atm) and the specific absorptivity of the gas ε (for example in cm⁻¹ atm⁻¹). At low values of α ℓ , Eq. (2) approximates to a linear relationship as follows:

$$I \approx I_0(1 - \alpha \ell) \tag{3}$$

Fig. 1 shows a schematic diagram of a simple NDIR gas sensor. Typically, emission from a broadband source (such as a microbulb [21]) is passed through two filters, one covering the whole absorption band of the target gas (in the active channel), and the other covering a neighbouring non-absorbed region (the reference channel). Typical filter characteristics for $\rm CO_2$ measurement are shown in Fig. 2, alongside the gas absorption spectrum. Provided that the chosen active and reference channel filters do not overlap significantly with the absorption bands of other gas species present in the application, cross-sensitivity to other gases lies below the limit of detection. Fortunately for $\rm CO_2$ sensing the filters shown in Fig. 2 are spectrally located far from absorption bands of potential interferents such as water vapour or hydrocarbons at typically

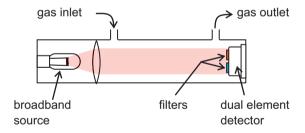


Fig. 1. Schematic diagram of a linear non-dispersive gas sensor with optical path-length in the range 3–20 cm. The source and detector are usually placed inside the cell to avoid baseline drifts that would otherwise be caused by variations in the background CO_2 concentration in the external optical path.

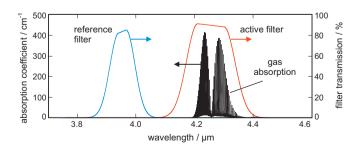


Fig. 2. Illustration of NDIR measurement principle. The absorption spectrum of CO₂ (calculated from the HITRAN database [22]) is superimposed on the transmission spectra of active and reference channel filters (approximated from ref. [7]).

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