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Item Type	Article
Authors	Salim, Mohd Rashidi;Yaacob, Maslina;Marcus, Tay Ching En;David, Michael;Hussin, Nabihah;Ibrahim, Mohd Haniff;Azmi, Asrul Izam;Ngajikin, Nor Hafizah;Dooly, Gerard;Lewis, Elfed
Citation	Jurnal Teknologi;73 (3), pp. 63-67
Publisher	Penerbit Universiti Teknologi Malaysia Press
Download date	2026-04-22 09:18:34
Item License	https://creativecommons.org/licenses/by-nc-sa/1.0/
Link to Item	https://hdl.handle.net/10344/8930

Analysis of Optimized and Improved Low Cost Carbon Dioxide (CO₂) Reflective Mid-Infrared Gas Sensor

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Article history

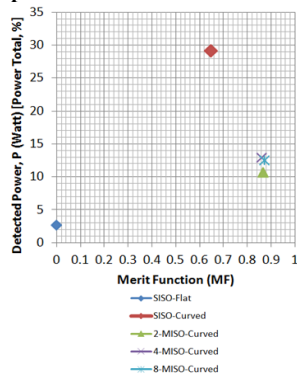
Received :15 August 2014

Received in revised form :

5 January 2015

Accepted :10 February 2015

Graphical abstract



Abstract

The optimized structure of CO₂ gas sensor has been simulated consists of low cost components and easy for fabrication. The structure is based on reflective type gas cell using aluminium material. Optimization was made on radius of aluminium surface to enhance the performance of the sensor. The results show that the gas sensor is fully optimized and able to detect higher power efficiently. It is proven that the optimized CO₂ gas sensor of 8-Multiple-Input-Single-Output (MISO) has capability to gain power of at least 1.0 Watt with 12.5% efficiency. However, Single-Input-Single-Output (SISO) has shown greater efficiency as it can detect 29.1% of total power supplied with the lowest Merit Function (MF) value of 0.648.

Keywords: CO₂; Reflective gas sensor; mid-infrared; power detection; efficiency; optimization; ZEMAX

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1.0 INTRODUCTION

Nowadays, modern industrialized society has not only brought to the world numerous goods and services, but also a series of problems related to technological development. Ever-increasing industrialization makes it absolutely necessary to constantly monitor and control air pollution in the environment such as in factories, laboratories, hospitals and generally technical installation¹. In recent years, several types of gases especially CO₂ has been used in different areas²⁻⁴. In fact, in many industries, gases such CO₂, Carbon Monoxide (CO) and Nitrogen Dioxide (NO₂) have become increasingly important as raw material. For this reason among others, it has become very important to develop highly sensitive gas sensors to prevent accidents due to gas leakages, subsequently saving lives and equipment⁵⁻⁷.

It is absolutely beneficial to have such highly sensitive and low cost CO₂ gas sensors for many applications mentioned above. An optimized CO₂ gas sensor has been developed using optical and

illumination design software, ZEMAX software to observe its performance such as gained power and level of sensitivity. This design is using low cost components and can be applied in harsh environment. In this project, non-sequential trace will be used as main technique to simulate the optimum structure of reflective gas cell. The design consists of few objects including Calcium Fluoride (CaF₂) window, curved aluminium surface, infrared light sources, detector and few types of tubes. Instead of using CaF₂ lens which price is much expensive as reported from previous researcher^{8,9}, it was replaced with CaF₂ window. The main purpose of window is to protect interiors of sensors and detectors from environment.

This proposed design of gas sensor is a reflective type gas sensor with highly reflective curved surface to reflect the transmitted light to a single detector. Optimization using Damped Least Squares (DLS)¹⁰ algorithm was simulated to determine the optimal radius of aluminium curved attached at the end of gas cell structure. Few simulations have been done using single and multiple filament emitters surrounding the detector to improve its

power detection level received. Several thickness of window were simulated to observe the changes if any. There are various types of tubes used in order to choose the best type of tube which includes compound parabolic concentrator (CPC), CPC rectangular, cone, cylinder tube, and rectangular tube. The simulation is based on the light source and detector of interest to ensure the practicality and the reliability of the design.

An optimized, compact and low cost CO₂ gas sensor has been successfully designed and analysed. In comparison to the previous works^{8,9}, the use of expensive material and component such as Chalcogenide Infrared (CIR) fibre¹¹ and CaF₂ lens¹² were replaced with lower cost component, such as CaF₂ window¹³. The CIR fibre is removed by attaching the emitters and detector directly on the surface of gas sensor. They are centered and located as close as possible in order to have better light coupling and reduce the loss due to scattered reflected light. Flat reflective surface is replaced by curved reflective surface to ensure more rays can be collected and focused on specified detector's channel, resulting higher power detection. Rather than using two ordinary detectors for CO₂ standard and reference as reported by previous researchers, this proposed design of CO₂ gas sensor using only a single multispectral detector¹² which already has two channels needed, hence make the overall design becomes more compact. Filament emitter used for this design has much better directivity based on its normalized output pattern as compared to previous emitter used due to built-in parabolic surface inside the emitter¹⁰.

2.0 MID-INFRARED COMPONENTS

2.1 Infrared Filament Emitter

In recent years, low cost and compact infrared filament emitters have been developed by many companies such as Ion Optics Inc.¹⁴ and Emitted Energy Corp.¹⁵ It is important to ensure that our design is robust, stable and capable of operating for long hours. Hence, it is highly recommended to use suitable components for the above mentioned characteristics. For light source, filament emitter from Ion Optics has been selected due to its great properties and advantages such as stable output, good directivity, robust, and able to transmit wavelength between 2 μm and 20 μm. Model Infrared filament emitter, ReflectIR-P1C is chosen as it has built-in parabolic structure, hence offers better directivity as compared to previously component used^{8,9}. Maximum power, maximum voltage and maximum current for this particular component are 1.7 Watts, 1.75 Volts and 0.97 Amps respectively.

2.2 Pyroelectric Multispectral Detector

Pyroelectric multispectral detector from InfraTec¹⁶ (LIM-262) is selected to be the detector of this design. It has dual channel, provided with TO39 housing, small chip size and thermal compensation. One channel is used for signal channel while the other one is used for reference channel. Suppose the reading interval of the gas cell is 200 ms. Then the bandwidth is 5 Hz. Based on its noise density¹⁶, the voltage due to noise is calculated to be 110.7 μV for 10 Hz bandwidth. Hence, the Noise-Equivalent Power is $110.7 \times 10^{-6} / 64000 = 1.73$ nW. So, the light power higher than 1.73 μW can be identified by the detector. Previously fabricated gas sensors⁸ used two detectors for reference and signal channels. By using this particular detector, there is only single detector is needed for both required channels. Pyroelectric detector fitted with a narrowband CO₂ filter centred at 4.24 μm with a 180 nm bandwidth and a reference pyroelectric detector centred at 3.95 μm with a 90 nm bandwidth.

2.3 CaF₂ Windows

It is a concern to develop such a low cost design. Hence, instead of using lens as previously fabricated^{8,9}, the lens was replaced with window. Window which can transmit light rays in a specific wavelength range with minimal distortions is important. Three limitations should be applied to a spherical window to minimize optical distortions such aperture (its largest dimension) should be smaller than the window's spherical radius, and thickness of the window should be uniform and much smaller than the radius. Reflective loss can be minimized by using antireflective coatings (ARC), which can be applied on either one or both sides of the window. These are the coatings that give bluish and amber appearances to photographic lenses and filters¹⁷. CaF₂ is often used in spectroscopic windows due to its high transmission from 250 nm to 7 μm. Its low absorption and high damage threshold makes it a popular choice to be used in numerous applications especially in this design¹⁸.

3.0 OPTICAL DESIGN OF GAS SENSOR

The optomechanical design of proposed gas sensor is shown in Figure 1. In comparison to transmissive type, a reflective gas cell is not only compact in size, but also offers better sensitivity due to its longer optical light path. It is proven from Beer Lambert law in which absorption is directly dependent on path length of the gas cell¹⁵. Initially, the pulsed infrared radiation from the filament emitter will be launched into the measurement chamber through CaF₂ window. Following transmission into the gas chamber, the infrared radiation travelled across 10 mm of cylinder tube where it will interact with the measurand gas before coming in contact with a curved aluminium end surface. Upon contact with the curved aluminium surface, parts of the infrared radiation will be transmitted back to the same CaF₂ window where it will be confined into the rectangular tube attached to centred pyroelectric detector. Hence, the infrared radiation will have propagated twice in the gas chamber to reach detector port. This will have indirectly doubled the total optical path length, subsequently resulting in better sensitivity.

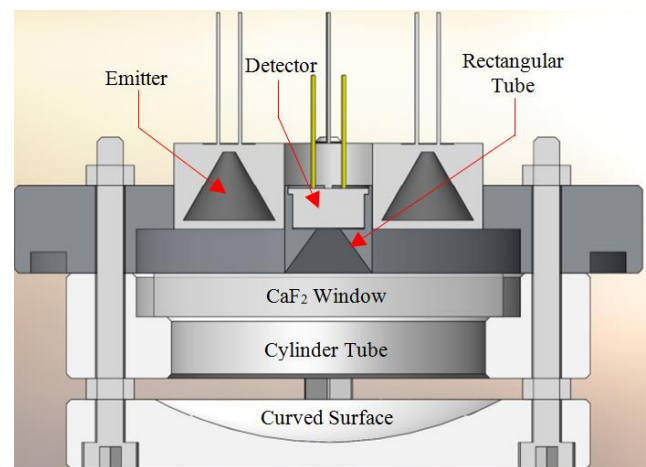


Figure 1 The optomechanical design of reflective gas sensor

As discussed in Section 2.1, ReflectIR-P1C¹⁴ was selected to be used in this proposed design due to more stable output and better directivity as compared to other models previously used. To simulate the actual selected infrared light source, we modelled the

ReflectIR-PIC in ZEMAX based on its normalized output pattern which can be found in its datasheet¹⁰ as tabulated in Table 1. Simulated normalized output pattern from ZEMAX for ReflectIR-PIC applied in this design is shown in Figure 2.

Table 1 Angle vs normalized output

Angle (degree)	Normalized Output
0	1
5	0.98
10	0.87
15	0.63
20	0.36
25	0.11
30	0.02
35	0
40	0

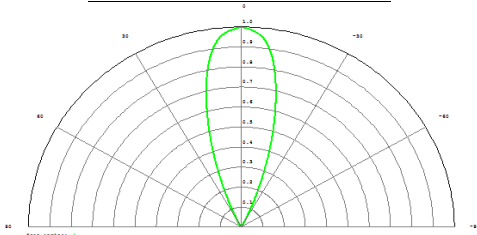


Figure 2 Simulated normalized output pattern of ReflectIR-PIC from ZEMAX

Figure 3 illustrates the ray tracing for non-sequential layout of few reflective gas cells. Notice that, multiple ray colours are used to show the ray propagation from one segment to another segment. Initial investigation was carried out using single-emitter-single-detector with flat and curved aluminium surface as shown in Figure 2(a) and (b) respectively. Ray tracing analysis was completed by using 10^6 rays before recording the total power detected. Further investigations were carried out using two-emitters-single-detector and four-emitters-single-detector as shown in Figure 2(c) and (d) respectively.

Optimization using DLS¹⁰ for each configuration was simulated to find the best radius of aluminium reflective surface. Optimization is the process by which a design is improved by changing the values of a set of parameters called variable such that the value of the Merit Function (MF) is reduced, or ideally driven to zero. In this design, the variable is the radius of the curved aluminium surface. The radius of curved surface will be optimized which could contribute to the highest detected power for each configuration illustrated in Figure 3.

DLS uses numerically computed derivatives to determine a direction in solution space which produces a design with a lower merit function. This gradient method has been developed specifically in ZEMAX for optical system design and is recommended for all optimization problems, such as optimization of radius of the curved aluminium surface in this proposed design. DLS has many attractive features; it is efficient, and it is very good at finding the "local" minimum of the merit function. In this context, the word local means the lowest value of the merit function that can be reached from the current position in solution space without ever increasing the merit function¹⁰.

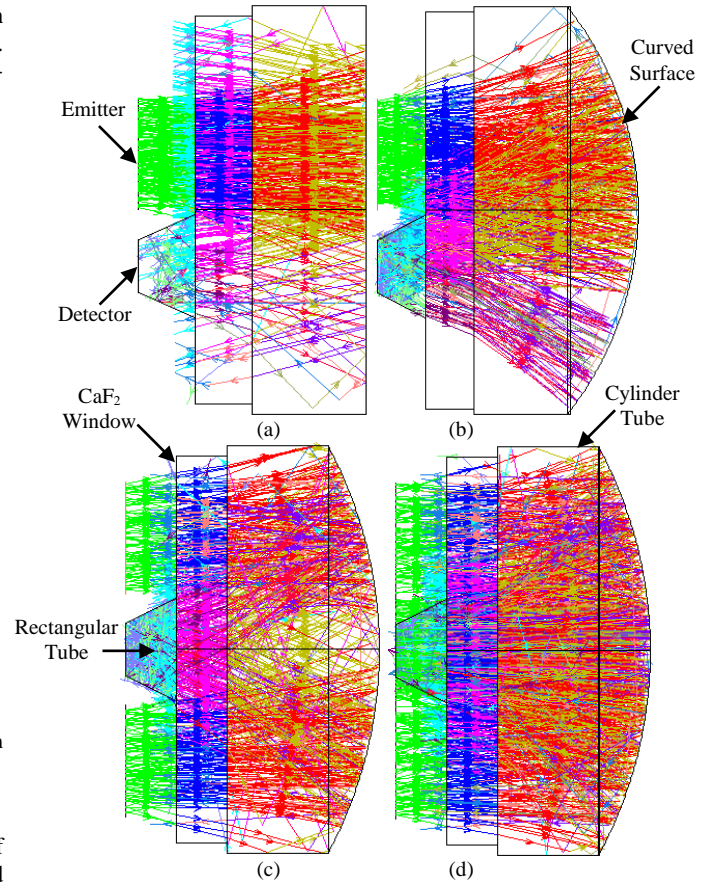


Figure 3 Ray tracing of reflective cell using single and multiple emitters; (a) SISO-Flat, (b) SISO-Curved, (c) 2-SIMO-Curved, (d) 4-MISO-Curved

4.0 RESULTS AND ANALYSIS

An optimized optical design using multiple emitters and single detector is illustrated in Figure 4. There are 8 filament emitters and single detector used in this design. The position of all filament emitters at (x,y): E₁(0,11), E₂(7.8,7.8), E₃(11,0), E₄(7.8,-7.8), E₅(0,-11), E₆(-7.8,-7.8), E₇(-11,0), E₈(-7.8,7.8) while the centered detector is positioned at D₀(0,0). From ZEMAX simulation using DLS algorithm¹⁰, the best radius of the aluminum surface has been optimized to be 42.11 mm. The diameter cylinder tube is set to 40 mm and has length of 10 mm. CaF₂ window¹⁶ with the thickness of 5 mm and diameter of 38.1 mm is antireflective (AR) coated for both sides. Rectangular tube has been designed in such a way that it could confine the transmitted light effectively to the required size of commercial detector's channel. In this design, the rectangular tube is placed between CaF₂ window and pyroelectric detector and has front size of 10x10 mm² and rear size of 2.7x5.2 mm². The length of the rectangular tube is set to 5 mm. Note that, simulated Sagittal depth, S is 5 mm as illustrated in Figure 4(a). Sagittal depth, S can be calculated and proved based on the following equation¹⁹.

$$S = R - \left[R^2 - \frac{D^2}{2} \right]^{\frac{1}{2}} \tag{1}$$

where R is the radius and D is the diameter.

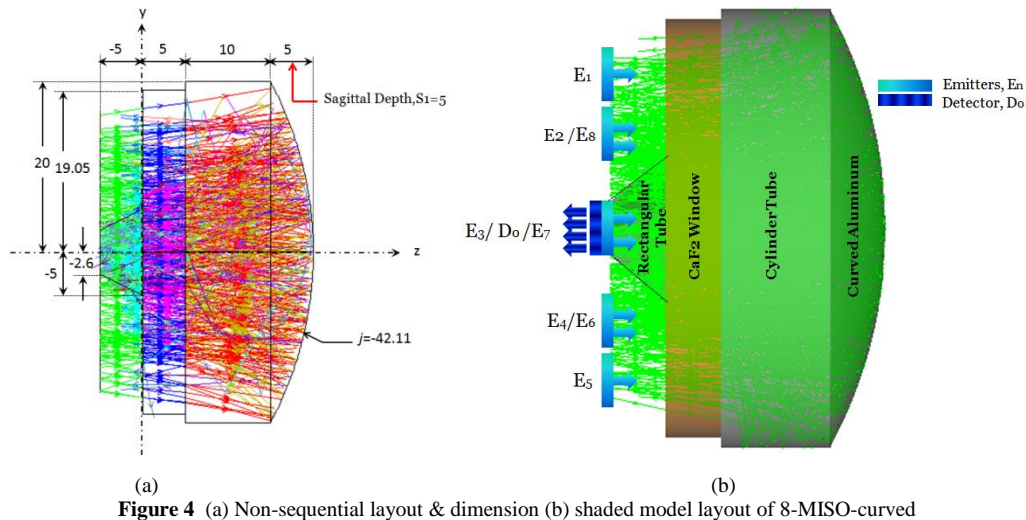


Figure 4 (a) Non-sequential layout & dimension (b) shaded model layout of 8-MISO-curved

Figure 4(b) illustrates the shaded model layout of 8-MISO-Curved. Table 2 shows the comparison on power detection for each configuration discussed. Power supply of each filament emitter used is set to 1 Watt. From the table, it can be seen that the SISO-Flat configuration has too much reflective loss in gas cell structure since the power received at detector is relatively small. Obviously the structure is not recommended for fabrication. 8-MISO-Curved configuration as illustrated in Figure 4 has superior detected power as compared to others. However, it has drawback in terms of efficiency. As can be seen from Table 2, 8-MISO-Curved has value of Merit Function pretty similar to others configuration and absolutely much higher than SISO-Curved has.

Figure 5 illustrates relationship between Power Detected (Watt) and Merit Function for each configuration. The lower value of Merit Function, the higher efficiency of the gas sensor as it has higher power detection. Even though the total power received by SISO-Curved is much less than received by 8-MISO-Curved configuration, it shows better performance in terms of efficiency with the lowest Merit Function value as shown in Table 2. Power efficiency can be calculated based on Equation 2:

$$P_{total}(\%) = \frac{P_{out}}{P_{in}} \times 100\% \quad (2)$$

Table 2 Comparison on detected power

Configuration	Total Input Power, P_{in} (Watt)	Optimum Radius (mm)	Merit Function (MF)	Detected Power, P (Watt)			
				Preference	P_{signal}	P_{out}	P_{total} (%)
SISO-Flat	1x1	N/A	N/A	0.0065	0.0114	0.0265	2.65
SISO-Curved	1x1	-36.29	0.648	0.0815	0.1161	0.2910	29.10
2-MISO-Curved	2x1	-42.18	0.866	0.0708	0.0710	0.2130	10.65
4-MISO-Curved	4x1	-42.06	0.860	0.1784	0.1772	0.5168	12.92
8-MISO-Curved	8x1	-42.11	0.872	0.3451	0.3453	1.0010	12.51

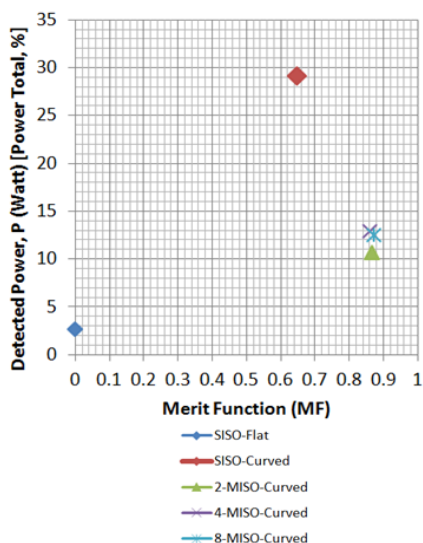


Figure 5 Graph detected power (Watt) vs merit function (MF) for each optimized configuration

5.0 CONCLUSION

The optimized optical designs of low cost CO₂ gas sensors have been successfully developed. The new design is the optimized and improved from previously fabricated gas sensor. The simulation is fully based on ZEMAX software, which provides the optimization tool for non-sequential optical system. Curved mirror has much greater ability to confine the reflected light to the allocated detected area as compared to flat mirror. Optimization using Damned Least Squares algorithm is used to simulate the optimum radius of curved surface. Total power received is direct proportional to the number of filament emitter used as the 8-MISO-Curved configuration has the highest level of power detection.

Despite the fact that total power received for SISO configuration with curved mirror is far less than received by 8-MISO configuration, it shows better efficiency. SISO with curved mirror is more efficient by having 29.1% of total input power and has Merit Function value of 0.648. Power received on signal and reference channels are 116.1 mW and 81.5 mW respectively. In conclusion, we would like to recommend both optimized optical designs, SISO-Curved and 8-MISO-Curved to be considered as optical gas sensor depending on sensing system's requirement. If the system with highest level of efficiency and lower cost is needed, then the SISO with curved mirror should be the best configuration to be considered. Meanwhile, the 8-MISO with curved mirror would be the best configuration for the required system with higher level of power detection.

Acknowledgement

The authors would like to acknowledge the support of the Human Capital Development, Universiti Teknologi Malaysia, Malaysia

and Ministry of Higher Education Malaysia for the scholarships given to the first author during the period of his study. A great appreciation is also dedicated to the STRoNG-TiES for the financial support given during the student mobility period of the first author.

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