

IMPROVING THE ACCURACY OF THE NDIR-BASED CO₂ SENSOR FOR BREATH ANALYSIS

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Abstract

The paper presents an analysis and practical study of the temperature and pressure influence on a non-dispersive infrared (NDIR) sensor for measuring the concentration of carbon dioxide in human breath. This sensor is used for monitoring patients' carbon dioxide (CO₂) in the exhaled air. High precision and accuracy of CO₂ concentration measurements are essential in air sampling systems for breath analysers. It requires an analysis of the influence of the human exhaled air pressure and temperature on the NDIR CO₂ sensor. Therefore, analyses of the changes in concentration were carried out at a pressure from 986 mbar to 1027 mbar and a temperature from 20°C to 36°C. Finally, corresponding correction coefficients were determined which allow to reduce the relative uncertainty of CO₂ sensor measurements results from 19% to below 5%.

Keywords: NDIR, CO₂ sensors, breath analysis, absorption spectroscopy

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1. Introduction

Analysis of the chemical composition of the human exhaled air is one of the novel non-invasive techniques in medical screening [1, 2]. More than 3000 different gaseous components have been found, so far [3]. Many of them are biomarkers with concentration (at the *ppb* - *ppm* level) corresponding to a specific disease. During exhalation, the biomarkers concentrations changes depending on a specific part of the human exhalation, so-called phases. The air from the gas exchange in the alveoli (phase III), containing the products of the body metabolic processes, is the primary source of medical data. One of the methods of this phase of selecting the part of the exhaled air is based on the analysis of changes in the concentration of *carbon dioxide* (CO₂). However, a high level of water vapor and changes in the exhaled air pressure and temperature may lead to erroneous measurements. Therefore, it is necessary to minimize these adverse effects to ensure the high precision of air sampling devices for the biomarkers analysis.

Changes in CO₂ concentration during exhalation are called a capnography waveform or capnogram [4]. The analysis of the waveform allows a separation of the exhalation into four phases. The analysed air in phase I is usually free of CO₂ and endogenous volatile organic compounds. In phase II, there is a rapid increase in the carbon dioxide concentration due to the increasing air from the alveolar fraction. During this phase, the contents of the alveoli are emptied. Phase III, also known as the "expiratory plateau", then begins with the maximum CO₂ concentration. The PetCO₂ point (partial pressure of the end-tidal CO₂) defines the end-expiratory phase (Table 1).

Tab. 1. Exhalation phases determined using exhaled CO₂ concentration [5].

Exhalation phase	Characteristics	Capnogram
I	Beginning of exhalation. Air from the upper respiratory tract not involved in gas exchange with blood	Low CO ₂ concentration (close to the atmospheric one)
II	Mixture of air from dead volume and alveolar air	Rapid increase of CO ₂ concentration (up to about 3% ÷ 5%)
III	Air from alveoli	Slow increase of CO ₂ concentration until it reaches its maximum value (PetCO ₂)
IV	End of exhalation and beginning of the next inhalation process	Rapid decrease in CO ₂ concentration to atmospheric air concentration levels

2. Research tasks and methods

2.1. Sensor analytical model

The purpose of analyzing the sensor performance in the absence of CO₂ is to determine the maximum power incident on the detector and to determine the ratio of the signal power to the noise power. Various sensors can be used to measure the carbon dioxide concentration, however, *non-dispersive infrared* (NDIR) type sensors are most commonly used in capnography [6–8] because of their selectivity, sensitivity, and rapid measurements [9]. The gas pressure and temperature changes can make a difference in the number of gas molecules and in the shape of absorption lines. The exhaled air is a compressible gas whose state is described by the equation:

$$PV = znRT, \tag{1}$$

where: P - gas pressure, V - gas volume, z - compressibility factor, n - number of gas moles, R - universal gas constant ($R = 8.314 \text{ J/mol}\cdot\text{K}$), T - gas temperature. Thus, the concentration of CO₂ in the exhaled air is directly proportional to the pressure and inversely proportional to the temperature of the air sample. This results in erroneous measurement results of the concentration. Therefore, a theoretical NDIR type CO₂ sensor model was developed to evaluate these errors.

The model idea is shown in Fig. 1. The sensor consists of a radiation source (RS), a detector (DET), and an optical filter (F). A gas sample (G) is analysed in a gas cell (GC) of the length L , where absorption of the radiation takes place at a specific range of wavelengths emitted from the RS, resulting in a change of an output signal (SIG).

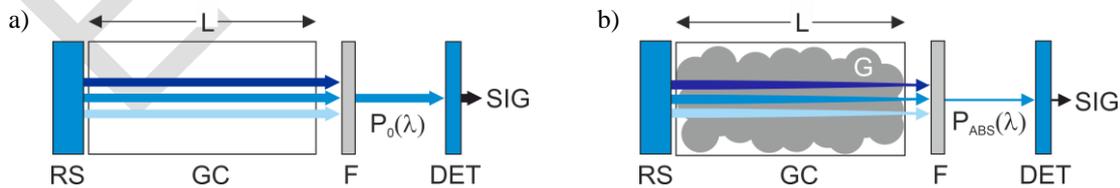


Fig. 1. Components of the NDIR sensor: $P_0(\lambda)$ is the radiation power incident on the detector with absence of gas in the gas cell (a), $P_{ABS}(\lambda)$ is the radiation power incident on the detector when test gas is present in the gas cell (b).

Detection is based on a comparison of two detector signals corresponding to the receiving optical powers for the empty $P_0(\lambda)$ and air-filled $P_{ABS}(\lambda)$ gas cell. The power of the radiation incident on the detector surface after passing through the gas can be determined from Lambert-Beer's law [10]:

$$P_{ABS}(\lambda) = P_0(\lambda) e^{-\alpha(\lambda)L}, \quad (2)$$

where: $\alpha(\lambda)$ - gas absorption coefficient determined as $\alpha = \sigma \cdot C$ (σ is the gas absorption cross section and C - gas concentration).

Parameters of the NDIR sensor model components for the spectral characteristics of determination of the radiation absorption were shown in Tab. 2.

Tab. 2. Main parameters of the NDIR sensor model components.

Component	Parameters	References
Radiation source	Centre wavelength $\lambda = 4.3 \mu\text{m}$ Radiation power $P \geq 0.3 \text{ mW}$ Beam divergence $\leq 50^\circ$	[11]
Gas cell	Cell length $L = 2 \text{ cm}$ Transmission range $\geq 4.1 \div 4.3 \mu\text{m}$	[12]
Optical filter	Centre wavelength $\lambda = 4.2 \mu\text{m}$ $FWHM \leq 120 \text{ nm}$	[13]
Radiation detector	Sensitivity range $\geq 4.1 \div 4.3 \mu\text{m}$ Normalized detectivity $D^* \geq 8 \cdot 10^{10} \text{ cmHz}^{1/2}/\text{W}$ Current responsivity $R_i \geq 1,3 \text{ A/W}$ Active area $A \geq 1 \times 1 \text{ mm}^2$ Time constant $\tau \leq 80 \text{ ns}$	[14]

Analysis of the absorption spectra was performed using the Hitran-PC software version 4.1 and the program database version 2008. Figure 2 presents the simulated results of the spectral characteristics of the transmitted LED radiation in a gas cell in two cases: empty (before absorption) and filled with the exhaled air. Analytical calculations enabled identification of the basic phenomena occurring in the NDIR sensor. The following assumptions were made in the calculations and subsequent analyses: the analysed gas is homogeneous inside the gas cell, there are no geometrical losses in the gas cell, no other gases, and apart from absorption, there are no other phenomena occurring in the tested gas (scattering, refraction).

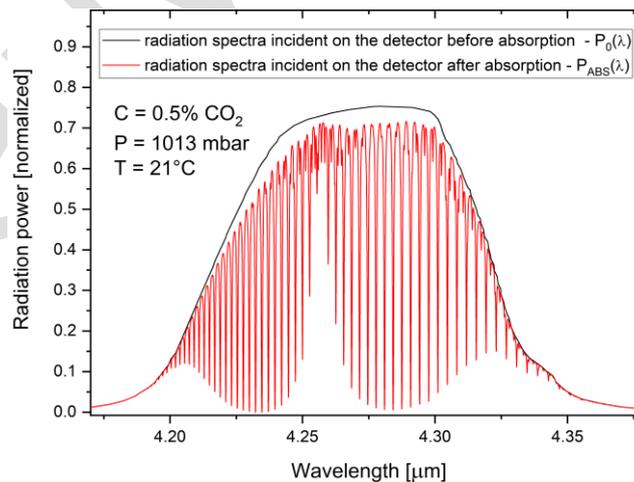


Fig. 2: Spectrum of LED radiation after passing through the empty (black line) and the breath-filled gas cell (red line).

The basis of physical phenomena in the sensor was analysed in the absence of the analysed gas in the gas cell ($\alpha = 0$) and in the presence of a 0.5% CO_2 concentration ($\alpha > 0$) inside the gas cell. For different pressures and temperatures, human exhaled air absorbance and *signal-to-*

noise ratio (SNR) were calculated to estimate the influence of these parameters on the NDIR sensor accuracy.

2.2. Analysis of the influence of pressure and temperature

The detector noise level was calculated. The RMS value of the thermal noise current I_{nt} was determined using the equation [15]:

$$I_{nt} = \frac{R_i(\lambda)\sqrt{\Delta f \cdot A}}{D^*}, \quad (3)$$

where $R_i(\lambda)$ is the spectral current responsivity and Δf is the detector noise bandwidth. The noise equivalent power (NEP) was calculated from the formula:

$$NEP = \frac{I_{nt}}{R_i(\lambda)}. \quad (4)$$

For noise bandwidth $\Delta f = 3.14$ MHz the values of these parameters are $I_{nt} = 2.9$ nA and $NEP = 2.2$ nW, respectively. Including LED radiation divergence, optical filter transmission, detector area and length of gas cell, radiation power incident on the detector will be $P_0 = 18.0$ nW, which generates the photocurrent I_f of 22.5 nA. Photocurrent will generate the shot noise I_{ns} , which can be estimated using the formula:

$$I_{ns} = \sqrt{2e \cdot I_f \cdot \Delta f}. \quad (5)$$

Estimated value of the shot noise $I_{ns} = 0.15$ nA. Signal-to-noise ratio can be expressed by the formula:

$$SNR = 20 \log \frac{I_f}{\sqrt{I_{ns}^2 + I_{nt}^2}}. \quad (6)$$

Determined SNR is ≈ 17.85 dB.

When a CO₂ sample is present in the gas cell, some of radiation will be absorbed by the gas. Based on the characteristics shown in Fig. 2, P_{ABS} will decrease to 17.2 nW. This means that there was a 4.4% decrease in the optical signal power due to absorption.

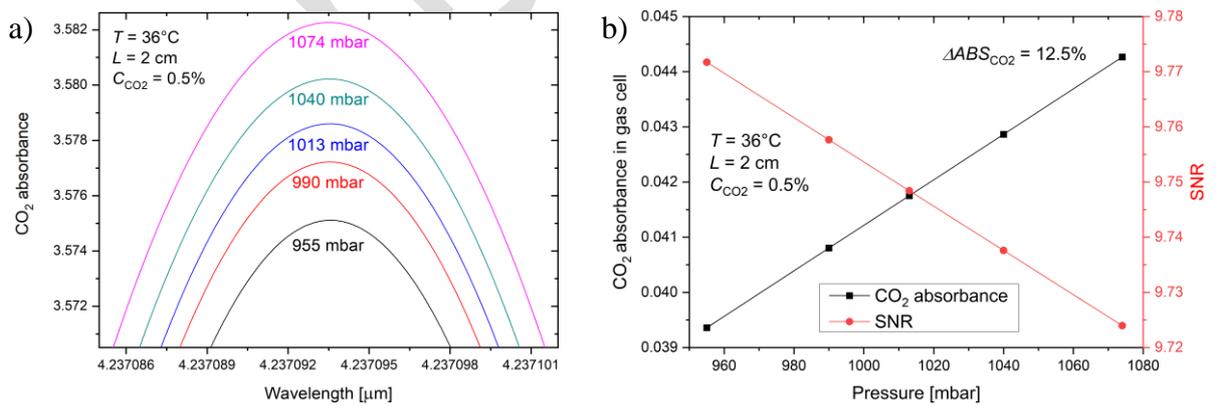


Fig. 3: Relationship between CO₂ absorbance on the sample absorption line (a) CO₂ absorbance in the gas cell and SNR (b) as a function of human exhaled air pressure.

Assuming air pressure conditions from 955 mbar to 1074 mbar and the fact that the pressure of the exhaled air should be 20 mbar higher than the atmospheric one [16], the analysis of the pressure influence in the range from 955 mbar to 1074 mbar was taken into account. Reducing the gas pressure, reduces its maximum value (Fig. 3a). The change in air pressure from the

minimum of the assumed range to the maximum causes an increase in the mean absorbance to the level of 12.5% (Fig. 3b). Consequently, it reduces the radiation power incident on the detector and reduces the output SNR from 9.77 to 9.72.

The influence of gas temperature from room temperature (about 20°C) to the maximum temperature of the exhaled air (about 36°C) [17] on the NDIR sensor output signal was analysed. Decrease in a gas temperature causes a decrease in the maximum absorbance value (Fig. 4a). However, an increase in gas temperature causes a decrease in gas absorbance to the level of 5.3% (Fig. 4b). Increasing gas temperature inside the gas cell increases the power of radiation incident on the detector leading to an increase in SNR from 9.72 to 9.75.

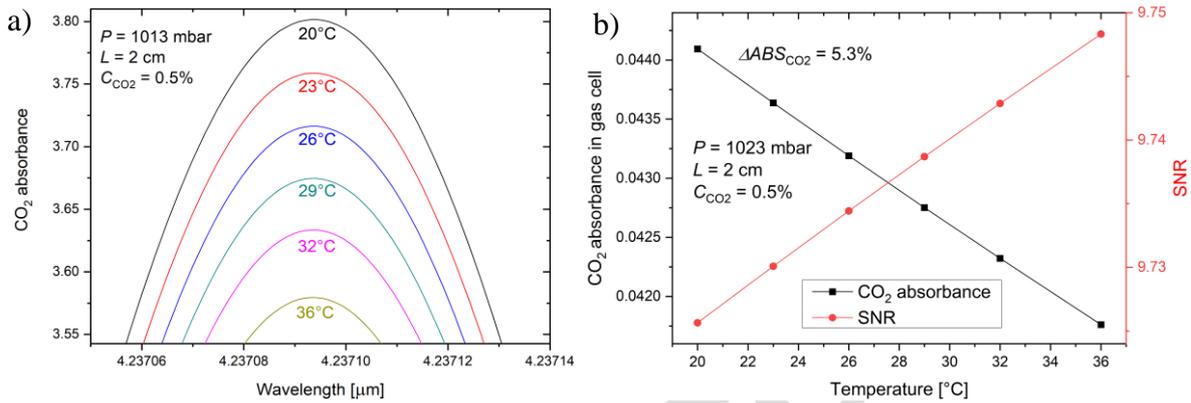


Fig. 4: Relationship between CO₂ absorbance on the sample absorption line (a) CO₂ absorbance in the gas cell and SNR (b) as a function of human exhaled air temperature.

As observed, the changes in gas temperature and pressure affect only the changes in gas absorbance, without significantly (about 0.3% ÷ 0.5%) affecting the SNR ratio. To summarize, increasing the accuracy of CO₂ concentration measurements with the NDIR sensor can be obtained by applying correction factors depending on the temperature and pressure of the tested gas sample.

3. Experiment

Theoretical analysis of the sensor model was experimentally verified using the UTECH UT100C sensor [18]. The MKS Type 1179A mass flow controller (MFC) was supplied from a cylinder with dry synthetic air of a 5% CO₂ concentration. Tests have been carried out from atmospheric pressure (986 mbar) to a pressure of 1027 mbar for the CO₂ sensor test below and above a standard pressure of 1013.25 mbar. Temperature was regulated using a universal oven model Memmert UF30 [19]. The BMP280 pressure and temperature sensor (absolute pressure accuracy of 1.0 mbar, absolute temperature accuracy of 0.5°C) was placed in the NDIR CO₂ sensor air stream, Fig. 5.

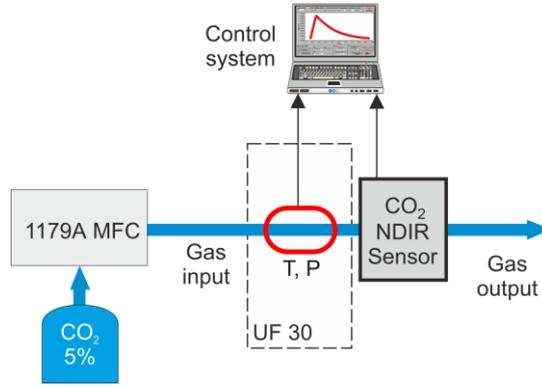


Fig. 5. Experimental setup for testing the CO₂ sensor. T – temperature sensor, P – pressure sensor.

Preliminary tests show that the humidity of the air sample did not affect the $\delta = 5\%$ uncertainty of the CO₂ sensor. Dependence of the NDIR sensor readouts when the pressure changes from 986 mbar to 1027 mbar is shown in Fig. 6.

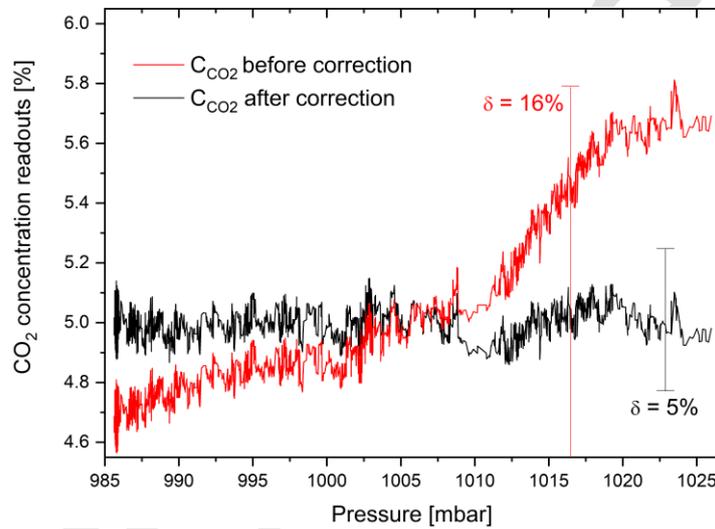


Fig. 6: Pressure influence on the UT100C CO₂ sensor readouts before and after correction.

The experiments confirmed that the CO₂ sensor measurements depend on the pressure of the flowing air. For low pressures, the sensor readouts were decreased while for higher pressures, sensor readouts were increased. Therefore, it was necessary to correct the sensor indications. The pressure (P) influence correction function was evaluated by an experimental approximation determined with the linear fit ($R^2 = 0.906$) by the OriginPro 2020 software and described by the formula:

$$C_{CO_2} = C_{SCO_2} \frac{208.2466}{P - 792.5177} \quad (7)$$

where: C_{CO_2} - CO₂ concentration after correction [%], C_{SCO_2} - CO₂ concentration before correction [%].

An analogous procedure was carried out to study the effect of temperature on CO₂ sensor readouts. A BMP280 sensor was used to measure the temperature. The results are shown in Fig. 7.

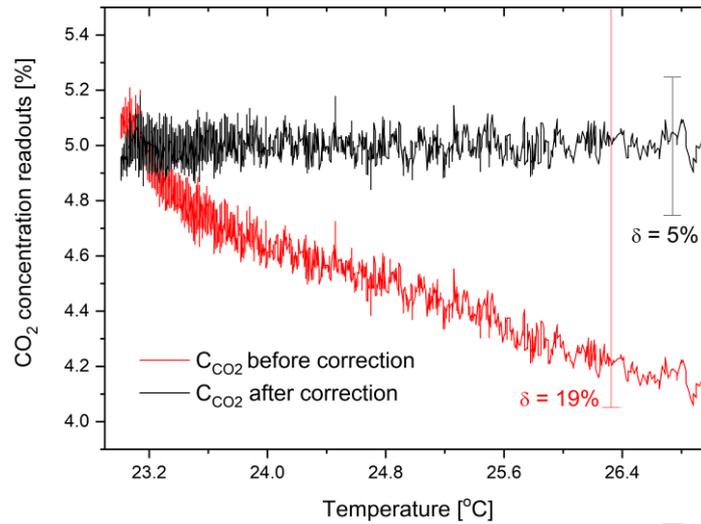


Fig. 7: Temperature influence on UT100C CO₂ sensor readouts before and after correction.

As the temperature increased, the CO₂ concentration measured with the NDIR sensor decreased at a rate of approximately 0.05%/°C. Therefore, the temperature (T) influence correction function was evaluated by the experimental approximation method determined with the linear fit ($R^2 = 0.883$) by the OriginPro 2020 software as:

$$C_{CO_2} = C_{SCO_2}(0.0102 \cdot T + 0.76212), \quad (8)$$

where: C_{CO_2} - CO₂ concentration after correction [%], C_{SCO_2} - CO₂ concentration before correction [%].

Based on the proposed CO₂ sensor readouts correction functions (7) and (8), correction factors were determined to minimize the impact of temperature and pressure on the UT100C carbon dioxide NDIR sensor readouts (Fig. 8). Thanks to this, the relative uncertainty of the sensor measurements was reduced from $\delta = 19\%$ to $\delta = 5\%$.

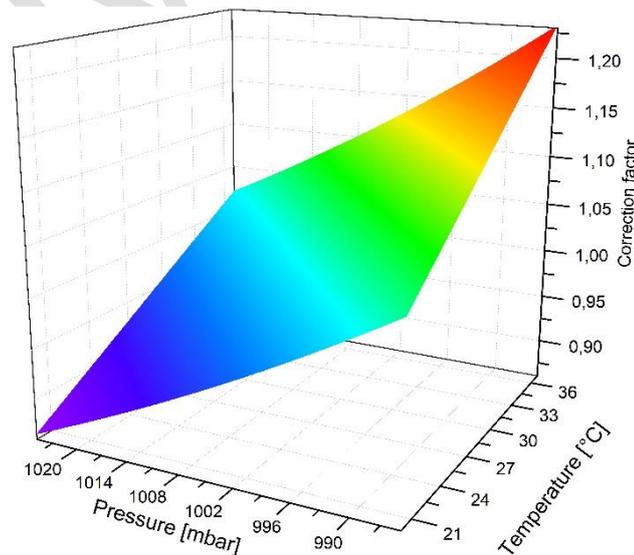


Fig. 8: Correction factors for pressure and temperature influence on CO₂ sensor measurements.

4. Conclusions

The NDIR type CO₂ sensors are commonly used for analysing the concentration of carbon dioxide exhaled by patients. However, the pressure and temperature of the air flowing through the sensor typically are not measured during breath, which leads to erroneous measurements. Since there is a need to accurately measure CO₂ concentration in devices for collecting and extracting specific phases from exhaled air samples, a correction of these measurements had to be performed with the NDIR sensor type. Influence was demonstrated theoretically and experimentally and the pressure and temperature correction factors were developed to reduce the relative uncertainty of the measurements with the use of a UT100C type CO₂ sensor from 19% to below 5%. Due to analogous phenomena occurring in other NDIR sensors, conducting a similar analysis should be taken into account.

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