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A Novel Real-time Carbon Dioxide Analyzer for Health and Environmental Applications

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Abstract

To be able to detect carbon dioxide (CO_2) with high accuracy and fast response time is critical for many health and environmental applications. We report on a pocket-sized CO_2 sensor for real-time analysis of end-tidal CO_2, and environmental CO_2. The sensor shows fast and reversible response to CO_2 over a wide concentration range, covering the needs of both environmental and health applications. It is also immune to the presence of various interfering gases in ambient or expired air. Furthermore, the sensor has been used for real-time breath analysis, and the results are in good agreement with those from a commercial CO_2 detector.

Keywords

carbon dioxide environmental analysis; breath-by-breath analysis; colorimetric sensor; end-tidal CO_2; capnography; respiratory diseases

1. INTRODUCTION

A capability that can detect carbon dioxide (CO_2) with high accuracy and with fast response time is critical for many health and environmental applications [1–15]. For example, measuring CO_2 levels in breath at the end of expiration, known as end-tidal CO_2 ($EtCO_2$), allows for non-invasive evaluation of systemic metabolism, perfusion, ventilation, and cardiac output, which provides doctors and patients with a non-invasive method to diagnose asthma, Chronic Obstructive Pulmonary Disease (COPD), and cardiovascular diseases [5, 6]. Similarly, monitoring of indoor CO_2 levels allows for assessment of indoor air quality (IAQ). Higher levels of indoor CO_2 are associated with increased prevalence of certain mucous membrane and sick building syndrome (SBS) symptoms [15]. Infrared detection technology is currently utilized for measuring CO_2 in breath and in air. While useful, this technology experiences strong interference from humidity that is present both in breath and in air. Moreover, the infrared approach requires special sample pretreatments in order to reduce the humidity, which further adds to the cost of the device technology and limits its usefulness for applications in clinical settings. In the case of indoor environmental CO_2

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sensing, the use of infrared technology is hampered by the interference of environmental humidity making detection of CO_2 levels inaccurate. There is a need, therefore, for developing a compact, low-cost, easy-to-use, and accurate CO_2 sensor for tracking CO_2 in human breath and for monitoring indoor air quality [16 – 17].

An alternative to infrared sensing is a detecting method based on colorimetry, which identifies CO_2 based on the change of color of a pH-sensitive indicator [18 – 23]. Compared to the infrared CO_2 sensors, the colorimetric approach has several potential advantages, including simplicity, miniaturization, low cost, and immunity to humidity changes, thereby making colorometric sensors an attractive technology. While these sensors may show great promise, their response and recovery time are too slow for breath-by-breath analysis, and their detection limits and reversibility are insufficient to ensure accurate detection of CO_2 in the environment. In order to solve these problems, many attempts, including pre-treatment of the sensing materials have been undertaken to reduce cost and ensure high performance of colorimetric CO_2 sensors. These improvement activities, however, often result in more complex instruments and sensor preparation methods.

In a previous publication, we introduced a portable breath analyzer for the determination of the expired CO_2. The device features a colorimetric sensor that could analyze breath CO_2 concentration accurately, and a fluidic system for efficient delivery of breath sample to the sensing element. A 3D model was created to simulate the sample flow and reaction of CO_2 with the sensing materials and color changes associated with the chemical reactions [24]. Despite the success, the sensor response was slow and semi-reversible, which is not suitable for breath-by-breath CO_2 analysis as needed for capnography, and moreover, which is insensitive to real-time monitoring of CO_2 in air. In the present work, we report a CO_2 sensor with a response time as fast as ~0.1 sec., which enables breath-by-breath analysis (see more details in Experimental and Results Section). Additionally, the sensor has a wide dynamic range (with the CO_2 concentration up to 11.5%), and low detection limit of a few tens of ppm, which are suitable for indoor air quality monitoring.

2. EXPERIMENTAL

2.1. Reagents and sensor preparation

The colorimetric CO_2 sensor presented in this paper was prepared by coating a sensor chip with a solution containing HCO_3^-/CO_3^{2-} buffer and *m*-cresol purple as the sensing element [19, 24]. All the reagents used in this work were analytical grade and purchased from Sigma-Aldrich (St. Louis, MO, USA). As described in our previous work, when an ambient air sample or warm breath sample was brought into contact with the sensor chip, the pH of the sensing material decreased, which led to a color change [24]. This color change was detected with an optoelectronic detection system (see details below).

Note that several differences are stayed in the present work with respect to previous work [24]. Regarding the sensor: **a-** The sensor substrate uses a fluorinated hydrophobic membrane instead of transparent polyethylene-based plastic; **b-** The hydrophobic membrane has microstructures and surface properties that provide faster water desorption and significantly improved sensor time response; **c-** The new indicator, m-cresol purple, provides a wider dynamic range of CO_2 % concentration due to its lower pka. Compared with thymol blue [24], *m*-cresol purple changes color more sensitively under weakly alkaline to neutral conditions (pH value: 9.0 – 6.0), which typically corresponds to the range of normal breath CO_2 levels (1.0% – 11.5%) [25 – 27] (Fig. 1).

Regarding the device: **a-** For breath applications, the gas flow is designed that both exhalation of breath samples, as well as inhalation of clean air are enabled through the

device. The later enables in-situ sensor regeneration; **b-** The device's gas flow component has larger diameter (~20 mm) than the device published in Ref. 24 (few mm), which significantly reduces the resistance to breathing, enabling breath-by-breath analysis.

2.2. Device description

The CO_2 sensor chip was inserted into a detection chamber, which included an optoelectronic detection system consisting of a red LED (wavelength = 633 nm, LEDtronics. Inc., CA, USA) as a light source and a photodiode (OSRM GmbH, Germany) as a light detector (Fig. 2a). The response of the sensor was characterized by measuring the change in the intensity of transmitted light caused by the interaction of CO_2 with the sensing element (Fig. 2b). Gas sample, from either the ambient air or a flow containing simulated breath was directed to the sensor detection chamber with a pump. Real breath test was also conducted by asking a volunteer to breathe into the device via a mouthpiece. The device also contains an electronic circuit, which collects and processes the data from the optoelectronic detection system, and then wirelessly sends the data to a smartphone via a Bluetooth chip.

2.3. Device characterization and validation

Simulated breath samples—In order to investigate the response of the CO_2 sensor to real breath, a humidified CO_2 gas mixture was employed to simulate the expired air. The simulated expired breath samples were prepared by first mixing 80% N_2 + 20% O_2 air with different amounts of CO_2 (Praxair. Inc.), ranging from 0.03% to 11.5%. The CO_2 mixtures were then pumped through a sealed water system immersed in a thermostatic water bath (Thermo Scientific, USA) at 35°C to generate 35°C and 100% relative humidity. The simulated expired gas samples and ambient air were then introduced into the breath analyzer alternately at a flow rate of 6L/min to simulate expiration and inspiration processes as shown in Fig. 3a.

Simulated environmental samples—For environmental CO_2 analysis, the CO_2 gas mixtures were prepared by mixing ultrahigh purity air with CO_2 to simulate indoor air with CO_2 concentration ranging from 0 ppm to 1350 ppm. The simulated indoor air samples and ultrahigh purity air were then alternately introduced into the CO_2 analyzer at a flow rate of 6 L/min as shown in Fig. 3b.

Sensor signal measurement—The change in light intensity of the CO_2 sensor was used to characterize the color change upon exposure to alternating sampling and purging periods of fixed time. The change in light intensity of the CO_2 sensor is evaluated as sensor signal from the baseline signal. This means that baseline shifts are corrected, which renders relatively small sensor response dispersion error at a given CO_2 concentration (see below for more details). The change in transmitted light of the CO_2 sensor is:

$$\Delta I(t) = I(t) - I(0),$$

where *I(0)* is the light intensity prior to the exposure of the sensor surface to the gas samples, *I(t)* is the light intensity at time *t* during the sampling process. In addition, the performance of this device was further validated using a commercial breath CO_2 analyzer (capnography analyzer from VacuMed, CA) and real breath samples from volunteers (Fig. 3c).

Cross-sensitivity analysis—The interference of other chemicals present in expired air and atmosphere, such as ethanol, acetone, acetonitrile, and NH_3 was investigated by introducing the humidified gas mixtures containing pure N_2 and the interfering gases into

the CO_2 analyzer. The response of the CO_2 sensor exposed to the interfering gases was compared with the response of the sensor exposed to 1% CO_2 gas mixture.

3. RESULTS AND DISCUSSION

3.1. Sensing mechanism of the CO_2 sensor

The basic sensing principle of the new CO_2 sensor is based on the adsorption and desorption processes of CO_2 in the sensor during the test [24]. Briefly, during the sensing process, as gas samples (either expired breath or environmental air) were introduced into the device, CO_2 was adsorbed by the HCO_3^-/CO_3^{2-} buffer system in the sensor, and the pH of the sensing system decreased. However, during the purging process, the clean air flowed over the sensor, and the CO_2 molecules were dissociated from the sensor, resulting in the recovery of pH to the initial value. As described in Section 2.1, *m*-cresol purple was used as the pH indicator of the sensing system. Since the variation of pH in the sensor was correlated to the concentration of CO_2 in the gas flow, the concentration of CO_2 in either the expired breath or environmental air can be determined via monitoring the color change of *m*-cresol purple (mCP). The chemical reaction process is as follows [28, 29]:

$$CO_2(g) \underset{k_0'}{\overset{k_0}{\rightleftarrows}} CO_2(aq) \quad \text{(R1)}$$

$$mCP^{2-}(purple)+H_2O+CO_2(aq) \rightleftarrows mCP^{2-}(purple)+H_2CO_3 \rightleftarrows mCPH^-(yellow)+HCO_3^- \quad \text{(R2)}$$

where $CO_2(aq)$ is the dissolved CO_2 in the sensor, mCP^{2-} is the deprotonated form of *m*-cresol purple and $mCPH^-$ is the protonated form of *m*-cresol purple in the HCO_3^-/CO_3^{2-} buffer solution.

3.2. Characterization of the CO_2 sensor

Breath CO_2 analysis calibration—Fig. 4a shows the response of the CO_2 sensor exposed to the alternating atmospheres of dry air and humidified 5% CO_2 gas mixture. As described earlier, when the CO_2 gas sample was introduced into the device, water vapor condensed onto the sensor surface and CO_2 was adsorbed by the HCO_3^-/CO_3^{2-} buffer solution in the sensor, which decreased the pH level of the sensing system, and changed the color of the pH sensing probe from purple to yellow (Fig. 2b). This color change was measured as a change in the transmitted light intensity, which was correlated to the CO_2 concentration in the gas sample. Conversely, when CO_2-free dry air was introduced into the device to simulate the inspiration process, CO_2 was stripped from the sensor and the color changed back from yellow to purple, which was also recorded by the light intensity change. The CO_2 concentration in the simulated breath sample can be determined from the maximum intensity change in each simulated breathing cycle. It is worthy to notice, the sensor signal noise at the maximum response level is generated by a current inability of the analog-to-digital converter of the microcontroller used in the detection system to smoothly manage small voltage signal changes. The problem is currently being corrected from hardware design standpoint. In addition, Fig. 4b shows the maximum light intensity change *vs.* the CO_2 concentration in the gas samples. It can be observed that the maximum change of light intensity increases with CO_2 concentration from 0.03% to 11.5% with a Langmuir-like behavior ($R^2 = 0.9986$). This concentration range sufficiently covers the need of breath CO_2 analysis for medical applications, which typically ranges between 2.5 and 5.0% in healthy individuals [30].

Environmental CO_2 analysis calibration—Fig. 5a shows the response of the CO_2 sensor exposed to the alternating atmospheres of ultrahigh purity air and simulated environmental air samples. The light intensity increased as CO_2 interacted with the sensing system and reduced gradually as pure air passed through the device. Fig. 5b shows the relationship between the maximum change of light intensity in each sampling-purging cycle and CO_2 concentration. The intensity change increased with CO_2 concentration with a Langmuir-like behavior ($R^2 = 0.9965$). The detectable range of the sensor to the ambient CO_2 was found from few tens of ppm to few thousand ppm levels, which covers the needs for environmental CO_2 detection [31].

3.3. Cross-sensitivity study

In order to investigate the interference effects of other chemicals that might exist in the expired breath and ambient air, humidified gas mixtures containing pure N_2 and different interfering gases were introduced into the CO_2 device at a flow rate of 6L/min for 30s. As shown in Table 1, compared to the response of the sensor exposed to a 1% CO_2 gas sample, the interference of the other gases is within 12%, which can be considered negligible in breath CO_2 analysis as the CO_2 levels in breath typically ranges from 3.5 to 5.5 %. However, interference from chemicals such as NH_3 needs to be corrected when the CO_2 sensor is used for environmental CO_2 monitoring.

In addition to the above-mentioned studies, the effect of ambient humidity on breath CO_2 analysis was evaluated. For relative humidity ranging between 20 and 85 %, the sensor response to the expired CO_2 remained constant within 10% variation (not shown). Some interference effect was detected for the relative humidity levels higher than 85%. However, the responses of the sensor to humid air and humid air with CO_2 mixture (e.g. simulated breath at 35°C, and 100% humidity) are different. Therefore the effect of extremely high ambient humidity could be corrected by use of an internal humidity sensor in the CO_2 analyzer.

3.4 Real breath analysis

In order to investigate the application of the CO_2 sensor to real breath analysis, including breath patterns and ventilation rate, the CO_2 sensor was calibrated using breath samples in combination with flow rate measurements from an *in-situ* flow meter. The breath patterns of two volunteers were also analyzed. The volunteers included one healthy person and one asthma patient from the VA Medical Center, Phoenix, AZ. They were asked to breathe normally through the mouthpiece. The end-tidal CO_2 values (the maximal concentration of CO_2 at the end of expiration) were calculated and compared with the values assessed from a capnogram recorded with a commercial breath CO_2 analyzer (Fig. 6). The “capnogram” refers to a real-time waveform of CO_2 concentration in the process of respiration with gas samples taken from a sidestream port located a few millimeters away from the colorimetric sensor as shown in Fig. 3c. From Fig. 6a and 6b, it can be seen that the end-tidal CO_2 values measured by the new CO_2 analyzer were comparable to the values assessed by the commercial analyzer for both the healthy person and asthma patient. In addition, the capnogram obtained from the new CO_2 analyzer also showed good agreement with the commercial device. The 90% response time of the CO_2 analyzer was less than ~150 ms, which meets the requirements for breath-by-breath CO_2 analysis (< 200 – 300 ms). Furthermore, the new CO_2 analyzer showed faster response than the commercial analyzer, which had a fraction of a second delay in gas detection due to the aspiration of the gas sample from the sample site through the sampling tube (around 3 ft. long) and into its detection unit (infrared detection chamber) (Fig. 3c). It was evident that time response improvements were achieved in the new CO_2 analyzer due to the *in-situ* location of the sensor chip in the mainstream of the breath sample flow.

4. CONCLUSIONS

This paper describes the development of a pocket-sized CO_2 sensor for personal healthcare and environmental monitoring. The device has an integrated circuit and an optical-based detection chamber, which includes a colorimetric CO_2 sensor. The CO_2 sensor shows reversible response to CO_2 and a dynamic detection range from ~50 ppm to 11.5%. When compared to a commercial infrared capnography detector, the CO_2 analyzer shows fast response with a 90% response time of less than 150ms, which indicates that the CO_2 analyzer is suitable for breath-by-breath analysis. In addition, the CO_2 sensor shows accurate detection of CO_2 levels after non-linear calibration of the sensor response. The interference study indicates that other chemicals typically present in the expired breath and ambient air have negligible effects on the response of the CO_2 sensor. Compared with traditional CO_2 measurement technology, the new pocket-sized CO_2 analyzer allows for simple, fast, and accurate assessment of breath CO_2 levels, and breath CO_2 profiles for patients with COPD and asthma, as well as CO_2 levels in ambient air.

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Biographies

Di Zhao received her BS and MS degree in Materials Science and Engineering from Tongji University in 2006 and 2009, respectively. She is currently working towards her PhD in Chemical Engineering at Arizona State University under the supervision of Dr. Erica Forzani. Her research interests focus on novel colorimetric sensors for the detection of gas and biomarkers in human breath.

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Highlights

- A novel real-time carbon dioxide (CO_2) sensor for health and environmental applications is developed.
- The sensor shows fast and reversible response to CO_2 over a wide concentration range.
- The sensor is immune to the presence of various interfering gases in ambient or expired air.
- The sensor can be used for real-time breath analysis, and the results are in good agreement with those from a commercial CO_2 detector.

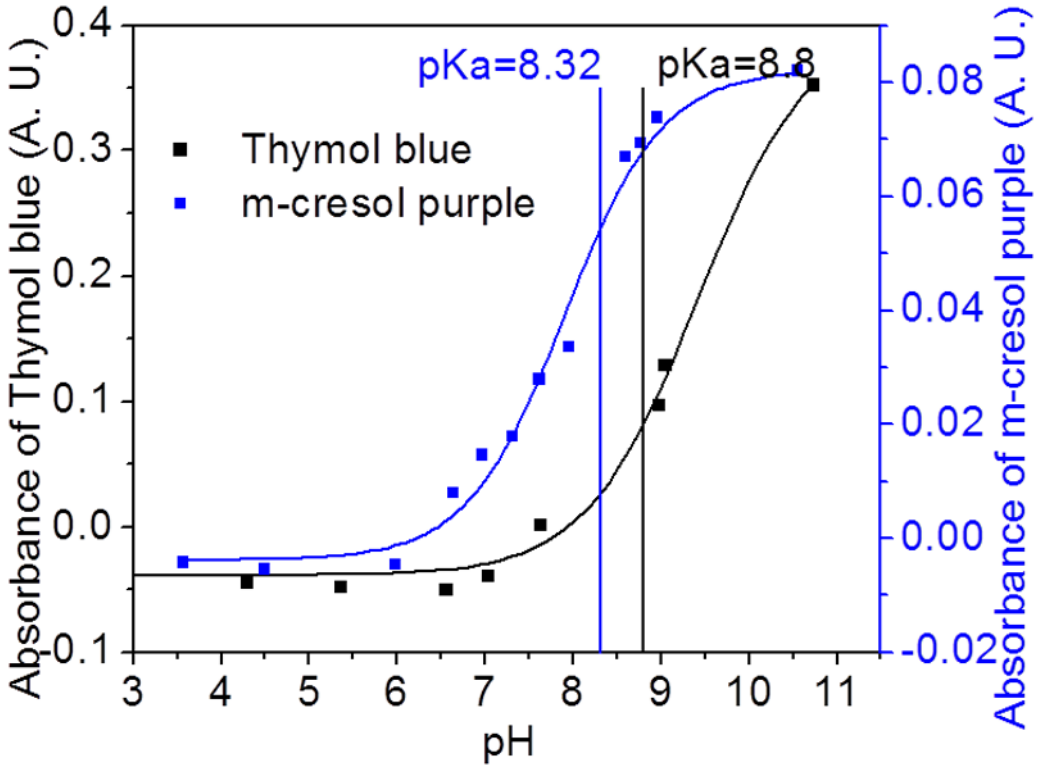


Figure 1.

Titration curves for the HCO_3^-/CO_3^{2-} buffer system modified with thymol blue and *m*-cresol purple. The color changes in the CO_2 sensor were due to the pKa value (for thymol blue: color changes from blue (pH > pKa) to yellow (pH < pKa); for *m*-cresol purple: color changes from purple (pH > pKa) to yellow (pH < pKa)). Compared with thymol blue, *m*-cresol purple changes color more sensitively under neutral to weakly alkaline conditions, which provides a larger dynamic range for the breath CO_2 detection.

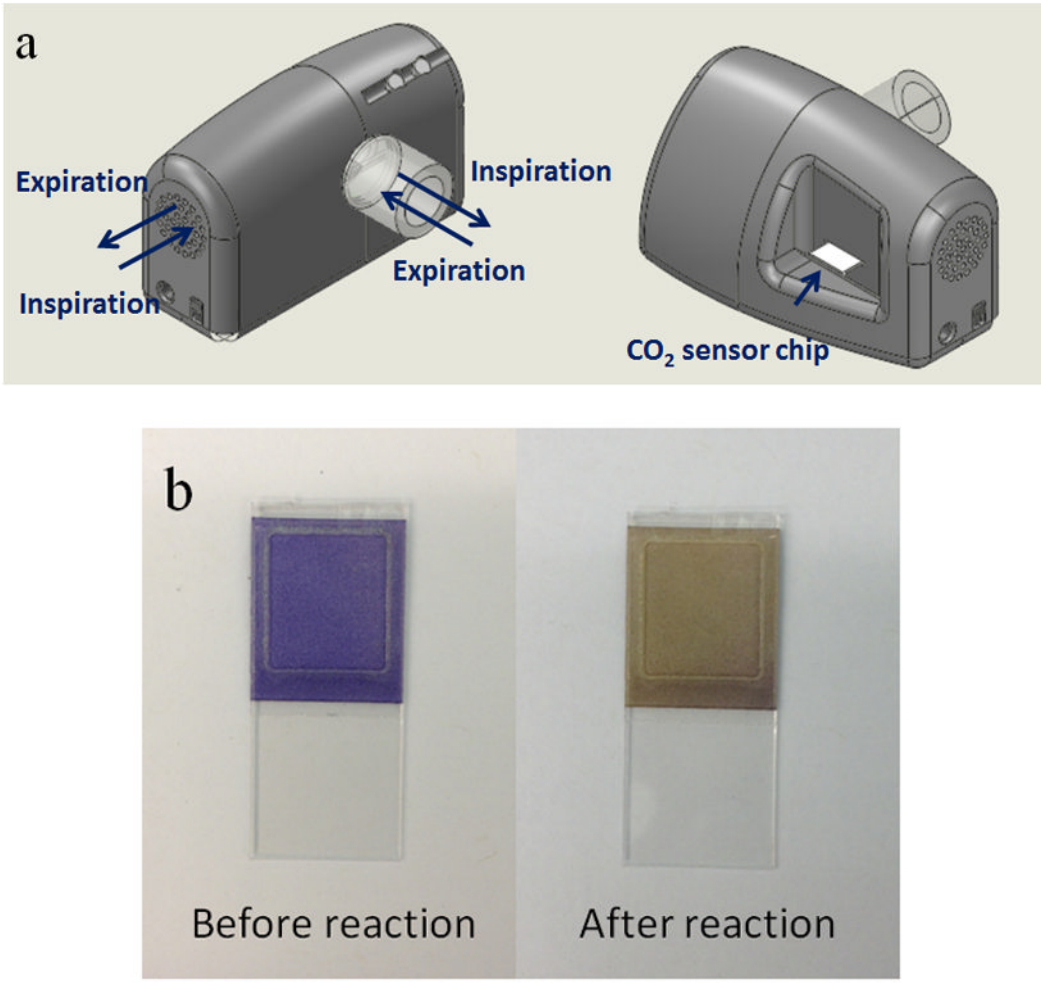
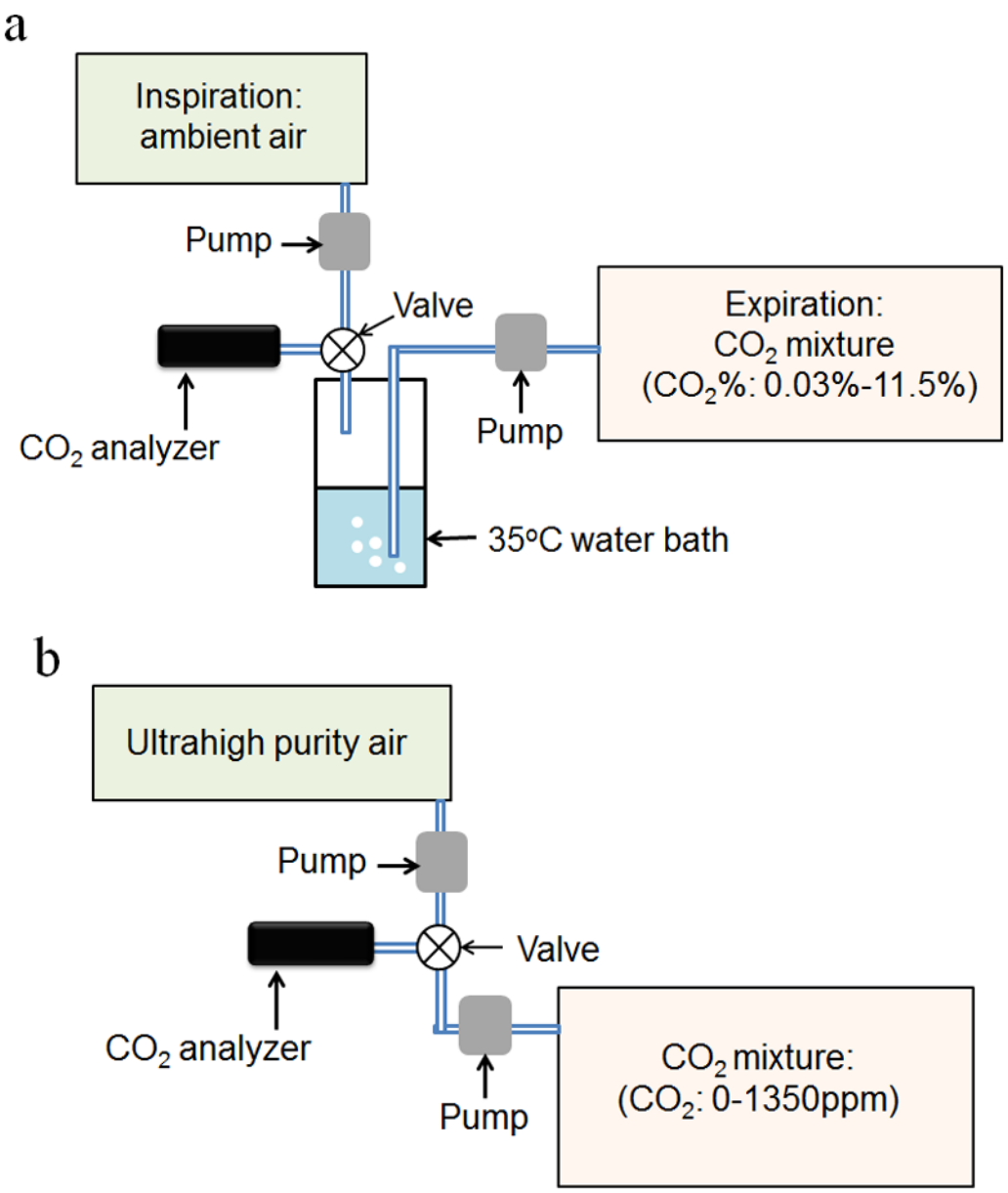


Figure 2.

(a) Pocket-sized CO_2 sensor device. It has inlets and outlets that allow the detection and analysis of both breath and environmental air samples. The key-sensing element is a CO_2 sensor chip, which can be inserted into or remove from the device. The device also features an electronic circuit for signal processing and Bluetooth for wireless transmission of data. (b) The sensor chip changes color from purple to yellow after exposure to CO_2 and the concentration of CO_2 is determined by measuring the change in intensity of transmitted light for the sensing element.



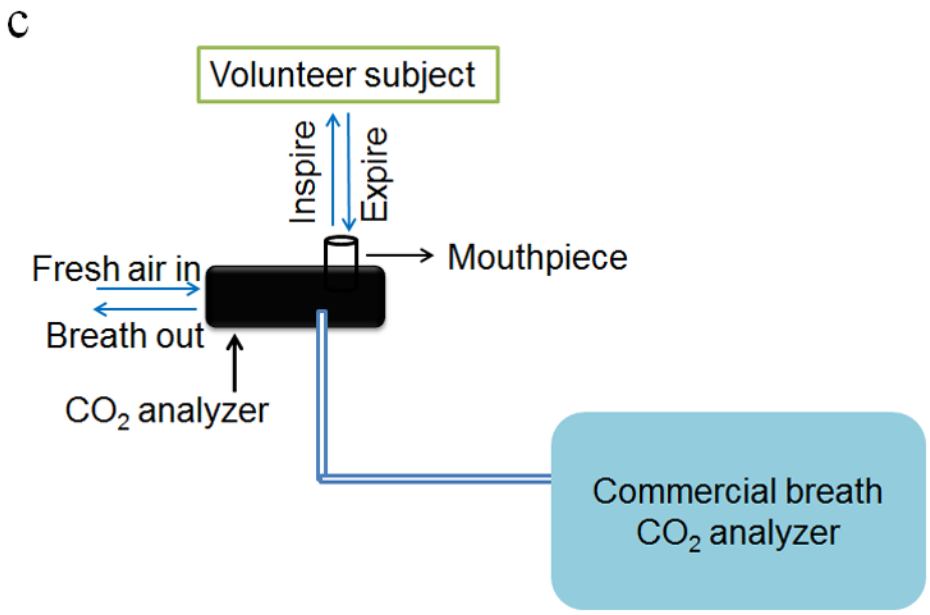


Figure 3.
Schematic diagram of calibration setup for investigating the response of the CO_2 sensor to (a) breath samples and (b) trace CO_2 in air gas samples. (c) Schematic diagram of the laboratory setup for validating the performance of the CO_2 sensor using real breath samples from volunteers and a commercial breath CO_2 analyzer.

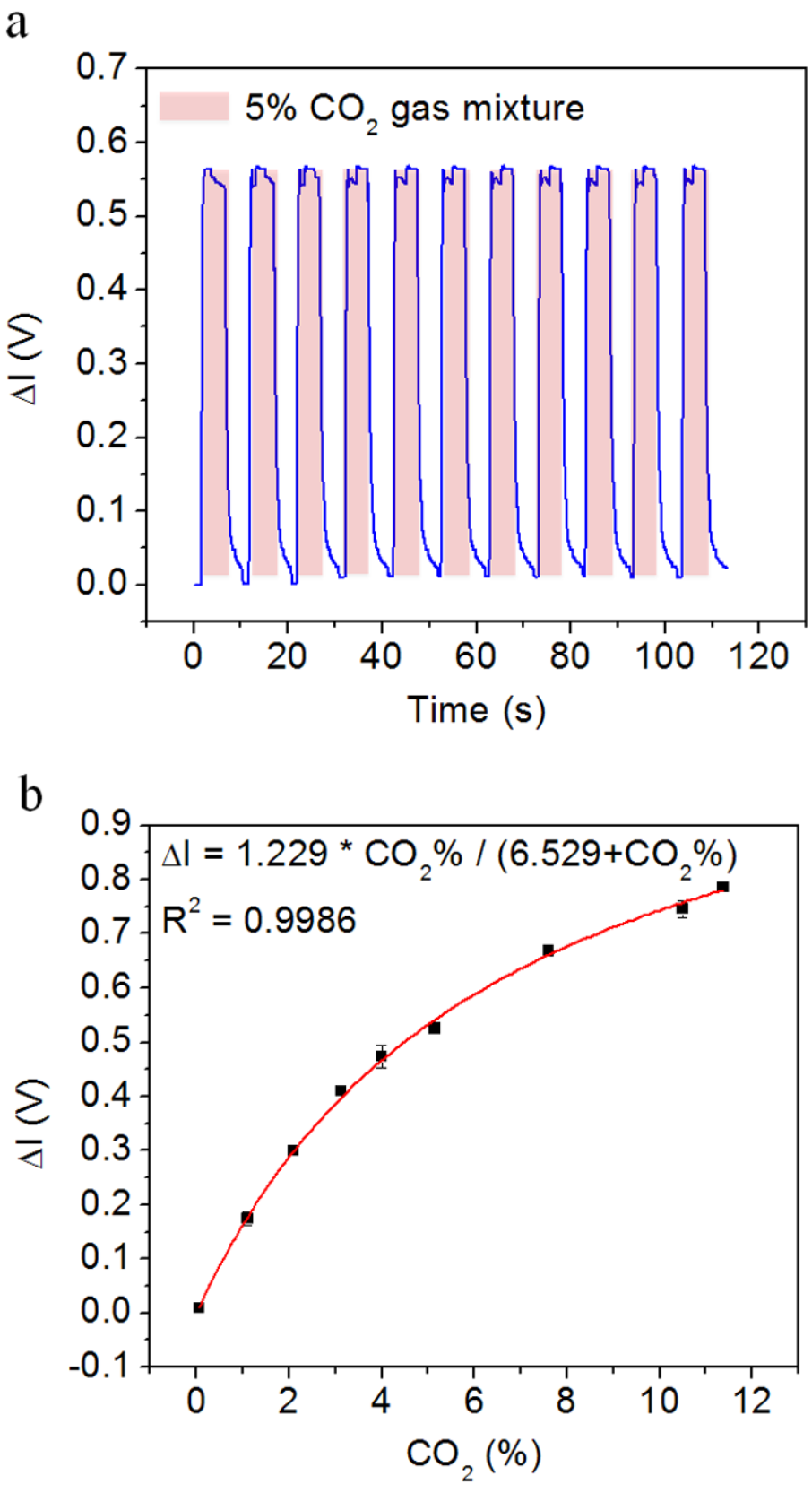


Figure 4.

(a) Response of the CO_2 sensor exposed to the alternating atmospheres of dry air and artificial expired air containing 5 % CO_2. The light intensity increases rapidly when the sensor was exposed to CO_2-containing atmosphere and returns to the initial value rapidly when the exposed to CO_2-free atmosphere. (b) The relationship between the maximum intensity change (indicated by ΔV, the output of the photodiode) and CO_2 concentration. The light intensity increased with the CO_2 concentration. Response vs. concentration to Langmuir-like equation is shown in the figure insert.

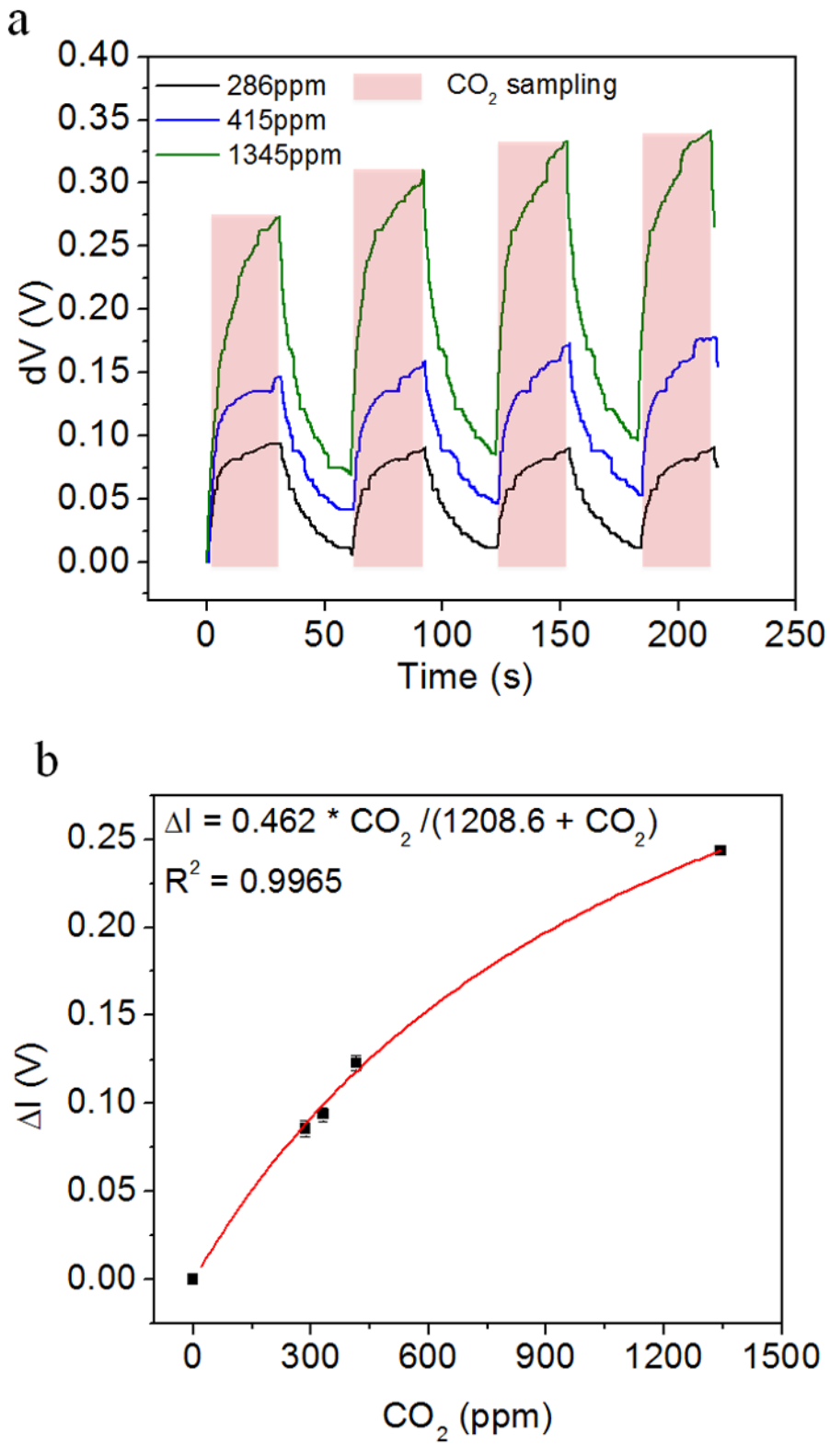


Figure 5.

Application of CO_2 sensor for environmental sensing: (a) Response of the CO_2 sensor exposed to the alternating atmospheres of simulated environmental air samples. (b) The light intensity changes increases with CO_2 concentration in the simulated environmental air sample. Response vs. concentration fitting to Langmuir-like equation is shown in the figure insert.

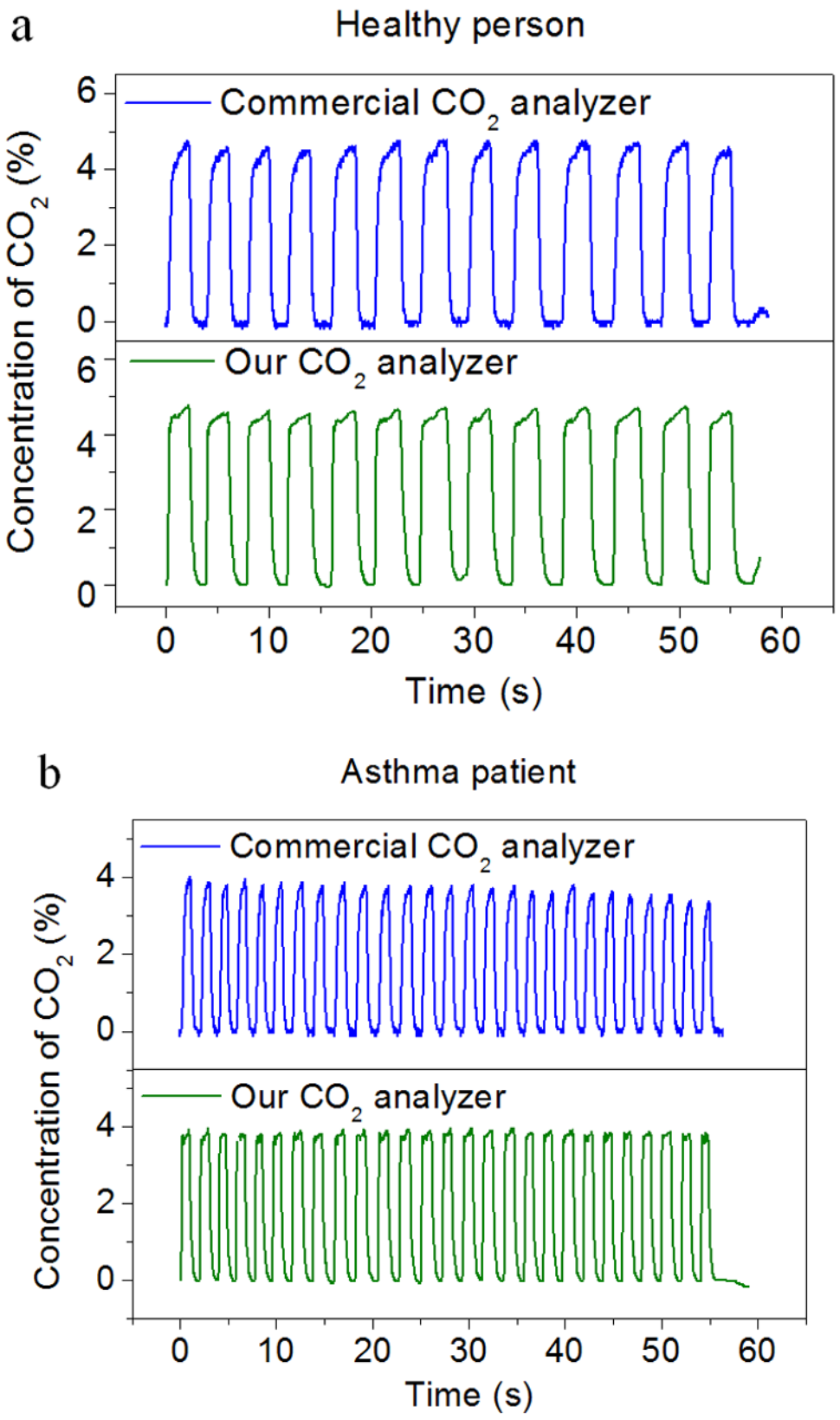


Figure 6.

Comparison of the CO_2 sensor by this work and a commercial infrared CO_2 analyzer. Both sensors were exposed to real breath samples from (a) a healthy person and (b) an asthma patient. The capnograms obtained from the present CO_2 sensor and the commercial device are in good agreement with each other.

Table 1

Cross-sensitivity of CO_2 sensor for other gases in the expired and environmental air

Gas	ΔI_{max} (V)	Maximum Interference (%)
1% CO_2	0.170	/
Pure N_2	0.010	5.8
165 ppm ethanol	0.014	8.2
20 ppm acetone	0.013	7.6
21 % O_2	0.017	10.0
250 ppb NH_3	0.017	10.0
100 ppb acetonitrile	0.019	11.2