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A personal device for analyzing carbon dioxide in real time and real breath: Experimental investigation and computational simulation

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ABSTRACT

The analysis of breath CO_2 provides valuable information of pulmonary and cardiovascular functions, and plays a crucial role in monitoring patients with respiratory problems. Developing portable sensors for real breath CO_2 analysis has been challenging because exhaled breath is hot, humid and turbulent. In this work, we have developed, modeled and tested a portable CO_2 sensor that can analyze end tidal CO_2 concentration in breath and in real time accurately. The key components of the sensor comprise a fluidic system for efficient breath sample delivery and a colorimetric detection integrated into the fluidic system. The modeling includes turbulent mass transport, heat transfer from the samples at body temperature to the device environment, and chemical reaction mechanisms, including multiple reactions pathways and diffusion of CO_2 in the sensing layer. Furthermore, the sensor has been tested and compared with a standard commercial CO_2 analyzer, and the results are in good agreement with those of the commercial analyzer, and with the modeling.

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1. Introduction

Among various chronic diseases, chronic obstructive pulmonary disease (COPD) and asthma are the leading concerns [1–5]. About 10 million Americans have been diagnosed with COPD and another ~20 million with asthma [5,6]. Breath carbon dioxide analysis is a well-known method that measures the breath CO_2 level, which is proportional to the partial pressure of CO_2 dissolved in blood [7–12]. The method is popular, effective and widely used to diagnose and evaluate the states of COPD and asthma, however, most of the current CO_2 equipment are based on infrared detection, which requires collecting breath samples with a pump, sample treatment to reduce interference from high breath humidity [13], and frequent calibration originated from signal drift. The high cost has also limited the use of current CO_2 equipment inside hospitals [14].

An alternative approach to measure CO_2 is based on colorimetric detection, which has been explored and developed by many groups with promising performance [15–20]. Nonetheless, in order to analyze CO_2 in real time and real breath (high humidity and temperature) without pre-conditioning of the sample, we need not only fast and accurate CO_2 sensor, but also efficient and reliable fluidic design that can deliver the breath sample from the mouth to the sensor, which remains unsolved in the existing colorimetric detections.

In the present work, we have successfully developed a low cost and high performance breath CO_2 analyzer for the personal use at home. The analyzer features an accurate colorimetric CO_2 sensor that can analyze end tidal CO_2 concentration in real time. More importantly, it includes a fluidic system designed for efficient delivery of breath sample to the colorimetric sensor. The integrated system, including both the sample delivery fluidics and CO_2 sensor, has been designed and optimized by carefully modeling and testing mass transport, heat transfer, and chemical reactions, such that we are able to achieve reliable analysis of real breath sample with high humidity and varying temperature. We believe that this integrated and system-level approach can be also applied to other types of chemical sensors for real breath analysis.

2. Experimental

2.1. Reagent and sensor preparation

The CO_2 colorimetric chemical sensor in the present work contained a HCO_3^-/CO_3^{2-} buffer and thymol blue as a color indicator

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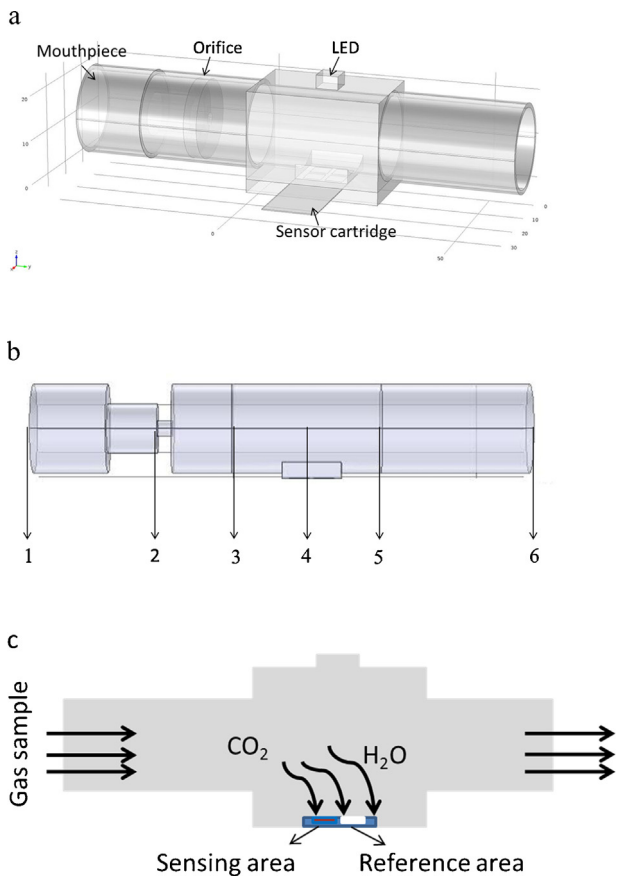

Fig. 1. (a) 3D geometry of the colorimetric CO_2 analyzer device and main device components. Simulated and real expired air was passed through the device from the mouthpiece. (b) Lateral view of the significant positions of the device indicated as follows: 1, inlet; 2, orifice (device narrowest portion); 3, middle portion between inlet and sensor chamber; 4, sensor chamber; 5, portion between sensor chamber and the outlet; 6, outlet. (c) Schematic representation of sample flow direction, and sensor cartridge components, showing the position of the sensing and reference areas.

[15–20]. All the reagents used in this work were analytical grade and purchased from Sigma-Aldrich (St. Louis, MO, USA). The sensor cartridge was made of a transparent plastic sheet, on which a sensing and reference areas were created (Fig. 1). The sensing area was coated with a solution containing HCO_3^-/CO_3^{2-} buffer and thymol blue, while the reference area was coated with HCO_3^-/CO_3^{2-} buffer only. The thicknesses of chemical coating layers for both the sensing and reference areas were determined to be a few hundreds of μm.

When the warm breath sample was brought into contact with the sensing cartridge, water vapor condensed on the sensor surface, forming a thin film of aqueous solution (see more details in later sections). Initially, the pH of the solution film was found to be ~9.05, but it decreased as CO_2 in the breath dissolved in the film. The pH decrease in the sensing area was detected by a color change of thymol blue from blue to yellow due to $pKa_2 \sim 8.0$–9.6 [15,16]. It is important to notice that the condensation of water plays role of hydrating the sensing chemicals and promoting the absorption of CO_2. In contrast, the reference area did not contain thymol blue dye and its color change was negligible, which served as a reference to correct drift in the color detection system.

2.2. Device description

The CO_2 analyzer is sketched in Fig. 1. It has a detection chamber, which includes a red LED (wavelength = 633 nm, LEDtronics. Inc., CA, USA) at the top of chamber as light source and a photodiode array (OSRM GmbH, Germany) at the bottom as light detector. The LED wavelength was chosen to closely match the absorption peak of Thymol Blue (615 nm). The detection chamber has also a sensor cartridge receiver located above the light detector. A sensor cartridge is inserted into the sensor cartridge receiver, and illuminated by the light source. The absorbance of the sensing area on the sensor cartridge is determined from the measured light intensities of the sensing and reference areas as a function of time, according to

$$Absorbance(t) = -\log_{10}\left(\frac{I_{sensing}(t)}{I_{reference}(t)}\right), \quad (1)$$

where $I_{sensing}$ and $I_{reference}$ are light intensities for the sensing and reference areas, respectively. Absorbance change is given by

$$\Delta Abs(t) = Absorbance(t) - Absorbance(0), \quad (2)$$

where $Absorbance(0)$ is the absorbance prior to the exposure of the sensor surface to breath sample. The measured absorbance change can be further normalized by the initial absorbance value, and it is the normalized absorbance change, Normalized $\Delta Abs(t)$, that is used to characterize the color change of thymol blue associated to CO_2 concentrations in the present work.

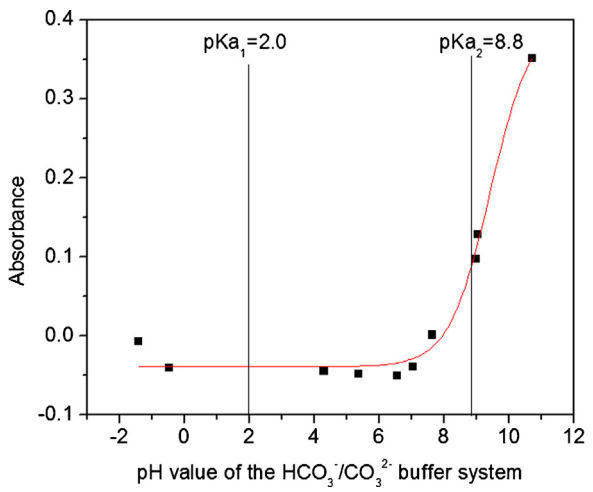

Fig. 2. The relationship between the measured normalized absorbance change and the pH of sensing HCO_3^-/CO_3^{2-} buffer system modified with thymol blue. The absorbance value increased with pH and followed a sigmoidal function: $Absorbance = 0.4 - \frac{0.4386}{1+\exp((pH-9.41085)/0.63016)}$. Values of p*K*a for thymol blue are indicated in the figure. Detected color changes in the CO_2 analyzer device were due to pKa_2 (with a color change from blue ($pH > pKa_2$) to yellow ($pH < pKa_2$)).

2.3. Device characterization – chemical characterization

Since the CO_2 detection is based on the pH change, which is measured from the color change, a calibration curve between absorbance change and the pH value is required, which was obtained by casting solutions of different pH values (measured with a pH electrode, Extech Instruments, NH, USA) onto the sensing area. The calibration curve, shown in Fig. 2, can be fit with a simple function,

$$Absorbance = 0.4 - \frac{0.4386}{1+\exp((pH-9.41085)/0.63016)}. \quad (3)$$

Using the calibration function by Eq. (3), one can relate the measured color change to the chemical reaction-induced pH change in the sensing area, which was needed for direct comparison between the measured color change and simulated chemical reaction taking place in the sensing area.