DOI 10.5162/eurosensors2026/3.1.2

Optimized Water-Based Colorimetric Carbon Dioxide Indicators for 455 nm Monolithic LED Emitter-Detector

Martí Verdaguer Mallorquí[1], María González-Gómez[1,2], Cristian Fàbrega[1], Joan Daniel Prades[2], Olga Casals[1]
[1] MIND/IN2UB, Dept. of Electronics and Biomedical Engineering, Universitat de Barcelona, Marti i Franqués 1, Barcelona ES08028, Spain
[2] Institute of Semiconductor Technology (IHT) and Laboratory for Emerging Nanometrology (LENA), Technische Universität Braunschweig, D-38106 Braunschweig, Germany;
mverdaguer@ub.edu

Summary:
A water-based m-cresol purple CO_2 indicator was optimized for sensing with a 455 nm monolithic LED emitter-detector platform. Printed films were evaluated under controlled CO_2 atmospheres using a commercial 455 nm LED setup. Single-factor and Design of Experiments studies identified individual and coupled formulation effects and supported selection of an optimized composition. Response models agreed well with an independently prepared formulation, and selected sensing layers produced clear concentration-dependent responses after integration on the monolithic device.

Keywords: Carbon dioxide, colorimetric sensor, m-cresol purple, blue LED, optical gas sensor.

Background, Motivation and Objective

Affordable CO_2 monitoring is increasingly relevant for indoor air-quality and ventilation assessment. Although nondispersive infrared sensors are widely used, their optical complexity and path-length requirements limit miniaturization [1]. Colorimetric indicators offer a complementary route by converting selective chemical interactions into measurable absorbance changes, but deployment requires stable films and compact electronic readout rather than bulky spectrophotometers, subjective visual inspection or illumination-sensitive camera methods [1,2].

This work builds on water-based m-cresol purple (MCP) CO_2 indicators, where CO_2 lowers the local pH and protonates the dye, producing a reversible optical change [3]. Water-based formulations are especially attractive because they have shown improved ambient lifetime compared with similar solvent-based indicators [3].

Recent compact colorimetric systems and water-based CO_2 inks demonstrate the relevance of this approach, but rely on different chemistries, device architectures or spectral ranges [1,2]. Here, the key challenge is matching the indicator to a monolithic blue LED emitter-detector platform operating near 455 nm. The objective is to adapt the water-based MCP formulation for 455 nm optical readout, enabling measurable CO2 sensing at reduced LED intensity and lower optical dose.

Description of the New Method or System

The proposed method is a device-constrained optimization of a water-based MCP CO_2 indicator for blue optical readout. Formulation variants are first printed on transparent polyester films and evaluated in a reference optical setup using a commercial 455 nm Oslon LED, selected to reproduce the emission range of the final device. The indicator film is placed between the LED and an IllumiaLite spectral flux analyser while controlled atmospheres with different CO_2 concentrations are generated. This setup allows the spectral transmission change of each formulation to be quantified under blue illumination.

The formulation is optimized by studying the amounts of the main indicator components: hydroxyethyl cellulose, glycerol, m-cresol purple and sodium bicarbonate. First, a one-factor-at-a-time approach is used to identify the individual influence of each component on the 455 nm response, response/recovery dynamics, film quality and stability. Then, a Design of Experiments approach is applied with hydroxyethyl cellulose held constant while sodium bicarbonate, glycerol and m-cresol purple are varied simultaneously. This links the chemical composition of the sensing film to the optical signal measurable at the wavelength of the target platform.

Selected formulations are then integrated on the monolithic emitter-detector LED device by spin-coating the indicator between the blue emitter and the matching blue receiver. In the final

sensor, CO_2-induced changes in the indicator absorbance modulate the blue light reaching the receiver and are measured as a change in the receiver signal. By maximizing the response at the available 455 nm band, the sensing layer enables measurable CO_2 readout at reduced LED intensity, thereby lowering the optical dose to the indicator.

Results

Formulation optimization focused on the optical response under 455 nm illumination, since this wavelength matches the blue LED emitter-detector platform. Measurements performed with the 455 nm Oslon LED showed that the water-based MCP indicator produces a clear CO_2-dependent decrease in transmitted blue flux, with the largest variation close to 450 nm. Complementary 2700 K white-LED spectra show that the dominant overall colorimetric change occurs around 590–600 nm, while a smaller CO_2-dependent feature is also present near the 455 nm region (Fig. 1). Together, these results show that the indicator can be read in the blue band, but that formulation optimization must be guided by the 455 nm signal rather than by the strongest broadband color change.

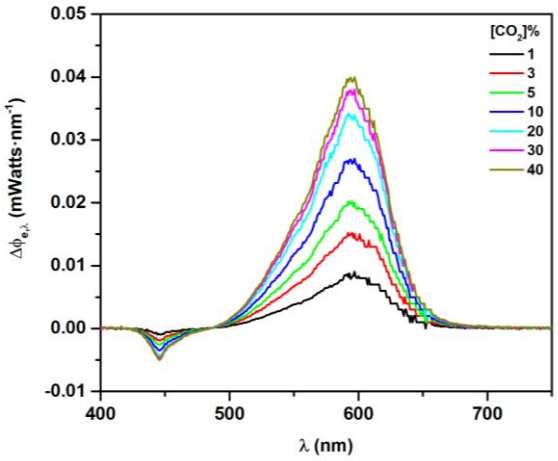


Fig. 1 CO_2-induced change in transmitted spectral flux of the water-based MCP indicator under 2700 K white LED illumination. The main spectral change occurs around 590–600 nm, while a smaller CO_2-dependent feature is observed near the 455 nm blue region.

The formulation study showed that the effect of composition depends strongly on the readout wavelength. This was particularly evident for sodium bicarbonate. Under 2700 K white illumination, lower bicarbonate content produced a stronger overall signal, with the lowest tested concentration giving the largest response. Under 455 nm illumination, sodium bicarbonate instead modified how the response developed across the tested CO_2 range: higher bicarbonate concentrations required more CO_2 to reach the same relative response. This confirms that formulations optimized from broadband or visual color change do not necessarily provide the most useful response for the blue LED platform.

The 455 nm one-factor-at-a-time study identified the individual role of each formulation component. Sodium bicarbonate influenced the response behavior and reversibility of the indicator. M-cresol purple increased the response amplitude, although excessive dye loading may compromise long-term stability by shifting the initial pH. Glycerol mainly affected response and recovery dynamics, while hydroxyethyl cellulose governed film homogeneity and processability with a weaker direct effect on the 455 nm response amplitude.

The Design of Experiments study was then used to evaluate coupled effects between formulation variables that could not be resolved by the one-factor-at-a-time study. In particular, the effect of glycerol on both response and recovery depended strongly on the sodium bicarbonate concentration. The DoE was also used to identify compositions that balance 455 nm response, recovery behavior, response across the tested CO_2 range and stability, and to construct response models relating formulation composition to the measured optical signal. These models showed good agreement with an independently prepared formulation.

After spin-coating on the monolithic emitter-detector LED platform, the selected sensing layers produced a clear concentration-dependent change in the receiver signal upon CO_2 exposure. This confirms that the formulation strategy developed under 455 nm reference illumination translates to the final blue LED readout configuration. By increasing the useful response at the available wavelength, the optimized indicator supports CO_2 sensing at reduced emitter intensity and lower optical dose to the sensing film.

References

[1] M. González-Gómez, I. Benito-Altamirano, J. D. Prades, O. Casals, and C. Fàbrega, Ultralow-Cost and Selective Water-Based Colorimetric Ink for Indoor CO_2 Monitoring, *IEEE Sensors Journal* 25, 18722 (2025); doi: 10.1109/JSEN.2025.3559593

[2] C. Driau, C. Fàbrega, I. Benito-Altamirano, P. Pfeiffer, O. Casals, H. Li, and J. D. Prades, How to implement a selective colorimetric gas sensor with off the shelf components?, *Sensors and Actuators B: Chemical*. 293, 41 (2019); doi: 10.1016/j.snb.2019.04.117

[3] A. Mills and G. A. Skinner, Water-based colourimetric optical indicators for the detection of carbon dioxide, *The Analyst* 135, 1912 (2010); doi: 10.1039/c000688b