atmosphere

Supplementary Materials for

Monitoring Tropospheric Gases with Small Unmanned Aerial Systems (sUAS) during the Second CLOUDMAP Flight Campaign

Travis J. Schuyler [1], Sean C. C. Bailey [2], and Marcelo I. Guzman [1,*]

[1] Department of Chemistry, University of Kentucky, Lexington, KY 40506, USA; travis.schuyler@uky.edu
[2] Department of Mechanical Engineering, University of Kentucky, Lexington, KY 40506, USA; sean.bailey@uky.edu
* Correspondence: marcelo.guzman@uky.edu; Tel.: +1-(859)-323-2892

Received: July 11, 2019; Accepted: July 24, 2019

The calibration curves S1, S2, and S3 for the methane (CH_4), carbon dioxide (CO_2), and ammonia (NH_3) gas sensors are provided below. Methane and carbon dioxide gas sensors were calibrated using primary certified gas and certified calibrated mass flow controllers. All concentrations are accurate within ± 1%. The gas sensors were calibrated in an environmental chamber where the gas composition, temperature and relative humidity were controlled.

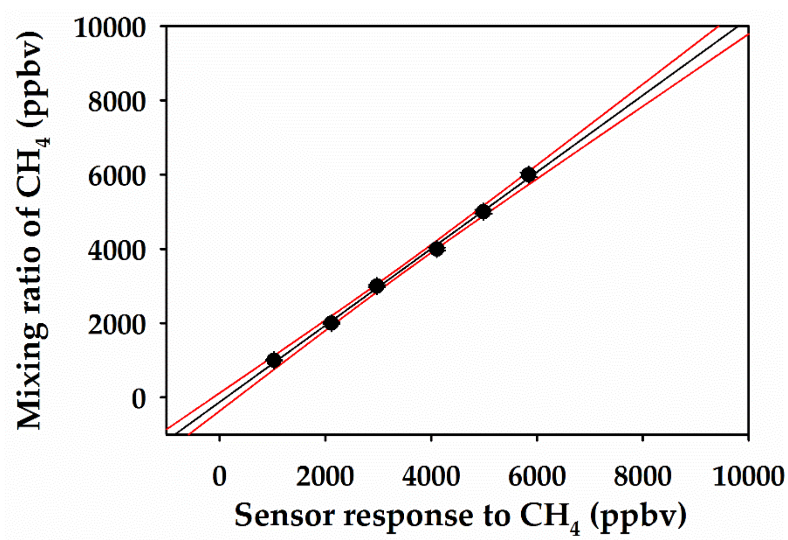

Figure S1. Methane calibration curve from 1000-6000 ppbv. y = 1.033(x) -122.0, where y represents the concentration of the gas of interest (in parts per billion by volume of air) and x the response of the sensor. The coefficient of determination for the straight line is $R^2 = 0.9981$.

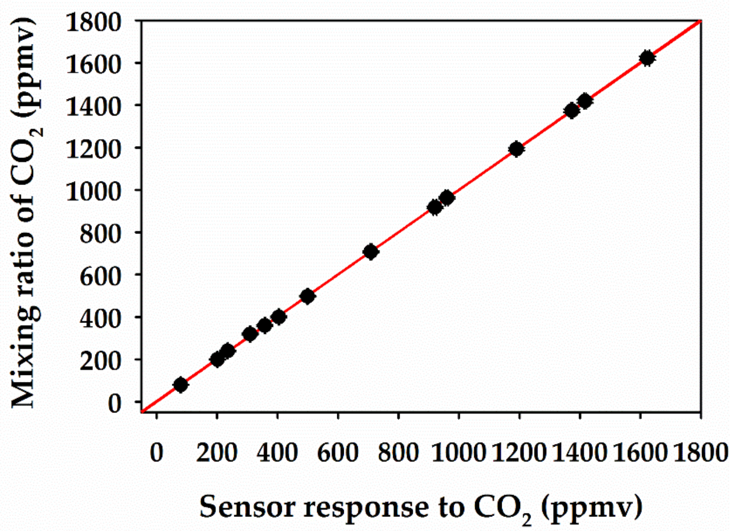

Figure S2. Carbon dioxide calibration curve from 80.00-1622 ppmv. y = 0.9993x – 1.682, where y represents the concentration of the gas of interest (in parts per billion by volume of air) and x the response of the sensor. The coefficient of determination for the straight line is $R^2 = 0.9999$.

The ammonia calibrations were achieved by using the custom environmental chamber. In brief, it is a sealed chamber that allows for total control of atmospheric composition. The ammonia vapor produced by ammonium hydroxide solutions of various volumes were used to calculate the theoretical ppbv of ammonia gas in the chamber. The stock ammonium hydroxide solution was 29.28%, or 15.45 M. Ammonium hydroxide forms ammonia and water as described in the acid base reaction below. The K_b of the reaction is provided in Equation 1.

$$NH_3(g) + H_2O\ (l) \rightleftharpoons NH_4^+(aq) + OH^-(aq) \qquad Reaction\ 1.$$

$$K_b = \frac{[NH_4^+][OH^-]}{[NH_3]} = 1.89\ x\ 10^{-5} \qquad Eqn\ 1.$$

The mole fraction of free NH_3 in solution was calculated using the pK_a and pH of the solution at 24 ˚C, and described in Equation 2.

$$NH_3(aq) = [10^{(pK_a - pH)} + 1]^{-1} \qquad Eqn\ 2.$$

Given that the pH of the 15.45 M stock solution was 11.60, 99.53% of the ammonium hydroxide was present as ammonia. Next, the partial pressures of ammonia and water were used to calculate the mass fraction of ammonia present as vapor above the solution. The fraction was multiplied by the mass of ammonium hydroxide in solution, and converted in μg. The mass was converted to ppbv by dividing the μg of ammonia vapor by the volume of the chamber in L to get ppbv. The calibration curve for the ammonia sensor is shown in Figure S3.

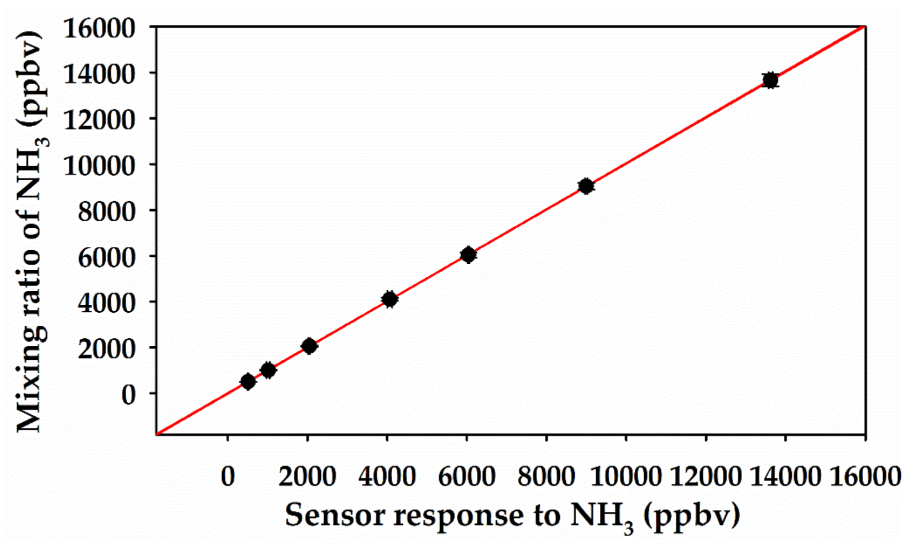

Figure S3. Ammonia calibration curve from 500.0-9040 ppbv. y = 1.003(x) – 0.0037, where y represents the concentration of the gas of interest (in parts per billion by volume of air) and x the response of the sensor. The coefficient of determination for the straight line is $R^2 = 0.9999$.

To test the effect of prop-wash on the sensor package, an experiment was designed to enable simultaneous boundary layer profiles (10-120 m) with a sUAS and tethered weather balloon equipped with the sensor packages. Figures S4-S8 compare the temperature, relative humidity, methane, carbon dioxide, and ammonia concentration data collected on board the sUAS (black line) and tethered balloon (red line). It is important to note that during the 2018 ISARRA LAPSE-RATE campaign, it was learned that the BME280 sensor (for temperature, pressure, and relative humidity) needs proper aspiration to be accurate [1].

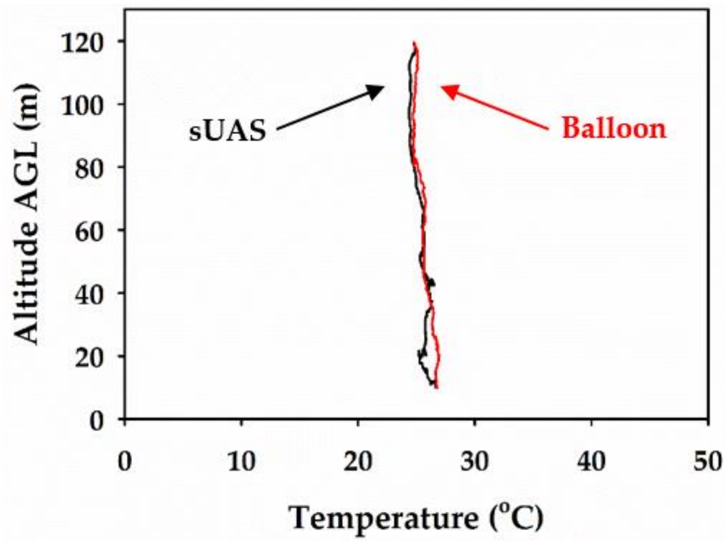

Figure S4. Temperature profiles AGL captured by a (black) DJI P3 quadcopter and (red) a balloon.

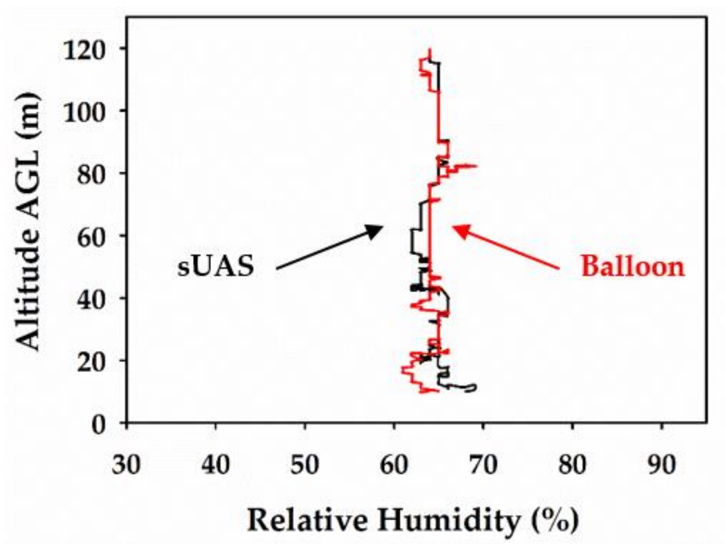

Figure S5. Relative humidity profiles AGL captured by a (black) DJI P3 quadcopter and (red) a balloon.

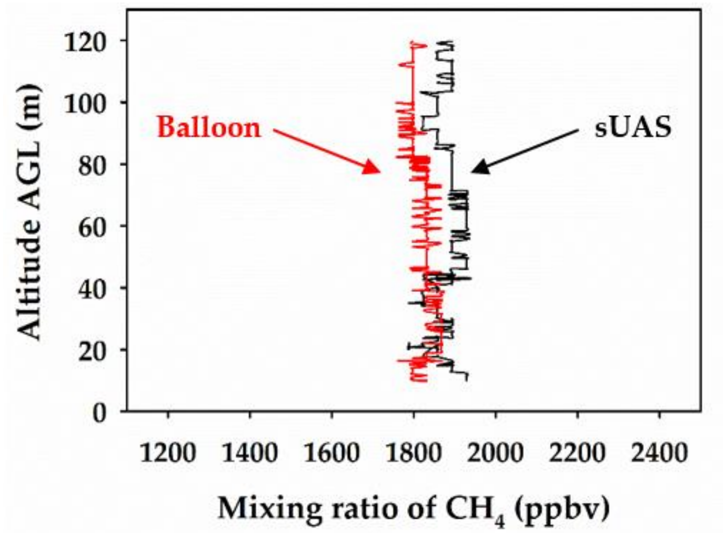

Figure S6 Methane profiles AGL captured by a (black) DJI P3 quadcopter and (red) a balloon.

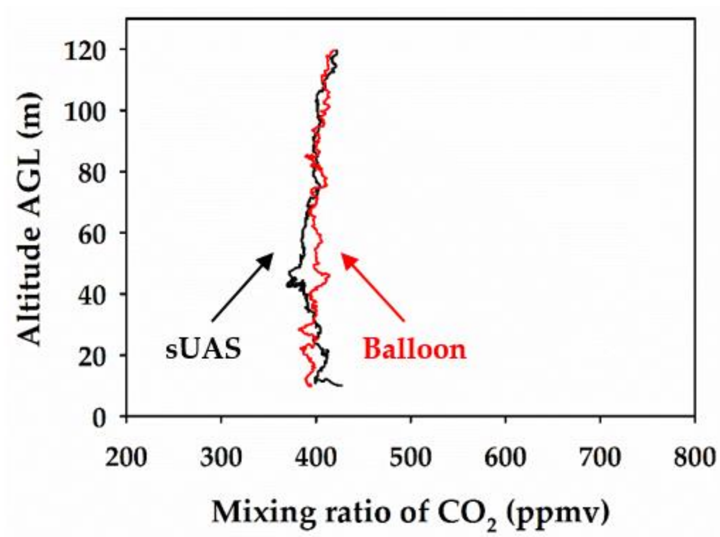

Figure S7. Carbon dioxide profiles AGL captured by a (black) DJI P3 quadcopter and (red) a balloon.

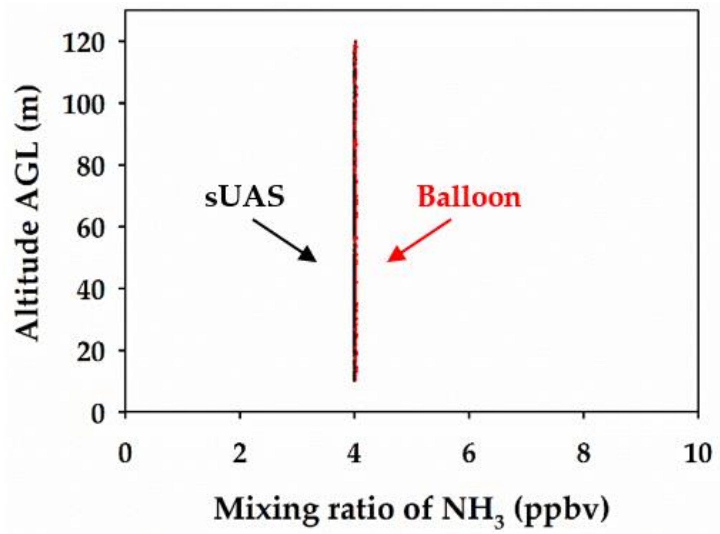

Figure S8. Ammonia profiles AGL captured by a (black) DJI P3 quadcopter and (red) a balloon.

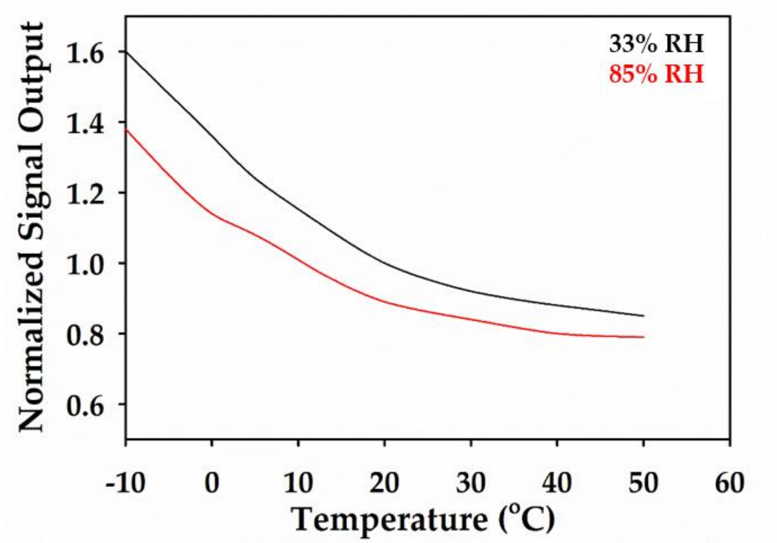

Figure S9. Calibration curve correcting the effects of temperature from -10 to 50 °C at low (33%) and high (85%) relative humidity [2].

This has been used as a starting place to successfully correct the sensor data for significant environmental changes. Corrections for the effects of extreme weather can be enabled in device software, or could be corrected after if absolutely necessary [2]. However, corrections for weather conditions are not needed for all sensors. For example, the MH-Z16 sensor for carbon dioxide measures its own temperature and uses that temperature measurement to provide a self-calibrated measurement. It is also unaffected by water vapor, so it does not needed to be corrected for different humidity's. Thus, there is no need for any corrections to the CO_2 sensor due to varying meteorological conditions.

References:

1. Barbieri, L.; Kral, S.T.; Bailey, S.C.; Frazier, A.E.; Jacob, J.D.; Reuder, J.; Brus, D.; Chilson, P.B.; Crick, C.; Detweiler, C. Intercomparison of small unmanned aircraft system (sUAS) measurements for atmospheric science during the LAPSE-RATE campaign. *Sensors* **2019**, *19*, 2179, doi: 10.3390/s19092179.

2. Hanwei Electronics. Specification Document for MQ-4 Gas Sensor. Available Online: https://www.pololu.com/file/0J311/MQ4.pdf (Accessed on 12 December 2016).