Miniature gas sensor for monitoring biological space environments

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ABSTRACT

A versatile gas sensor for use in gravitational studies and/or long-term monitoring of biological systems in space is described. The sensor combines two diode lasers in a compact, low power package for quantitative, simultaneous measurements of oxygen, carbon dioxide and potentially, water vapor. Wavelength modulation spectroscopy(WMS) combined with digital signal processor (DSP) control allows this system to meet the stringent weight and power restrictions of a space-borne sensor. The sensor, configured for measurements in plant growth chambers, exhibits a very high level of precision for long-term measurements, with an uncertainty in CO_2 concentrations of better than 3 parts per thousand (ppth), and about 5 ppth for ambient oxygen, all at 1 Hz. Allan variance measurements indicate that increasing the averaging time to 100 sec will improve the precision to 0.3 ppth. The dynamic range for CO_2 detection exceeds four orders of magnitude.

1. INTRODUCTION

A great variety of applications for space-based gas sensors exists, including uses for monitoring ambient oxygen levels, detecting buildup of harmful gases, detecting fire or smoldering events, for use in plant growth chambers, and additional research studies of combustion and biological processes. However, the spacecraft environment presents a number of challenges and constraints beyond those found in Earth-based systems. These include issues of weight, size, power, vibration and safety. Additionally, sensors must operate autonomously for extended time periods without need for recalibration. In this paper, we present results of research leading to the development of a space-based gas sensor using diode laser optical absorption wavelength modulation spectroscopy (wms). This approach is implemented with a fully solid-state control and analysis digital signal processor (DSP) system to provide multiple gas detection in real time that should meet the constraints required for space flight. In this instrument a distributed feedback (DFB) diode laser operating at 2000 nm is used for detection of carbon dioxide and a vertical cavity surface emitting laser (VCSEL) at 760 nm is used for molecular oxygen detection.

The pertinent design and operational issues and how we address them follows. A list of preliminary technical specifications is shown in Table I.

- Self-contained – The sensor must operate autonomously for extended periods without need for maintenance, recalibration, or operator intervention. DSP Microprocessor control assures that the sensor is always operating properly, automatically transmits/displays the required information and continuously performs internal health checks and identifies malfunctions.
- Ruggedness – The sensor is constructed entirely of solid state components, with no chemicals, cooling fluids, fragile components, or critical optical alignments required for robust operation
- Self-calibration – To assure long-term reliability, the sensor must be self-calibrating or, at a minimum, simply calibrated. One advantage of optical absorption is that the absolute concentration of the gas is directly obtained with the only variables being well-known spectroscopic constants, the modulation depth and path length. Fluctuations in the light source or optical alignment are automatically removed by an inherent ratiometric normalization of the laser intensity to 2*f* WMS signal.

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Diode Lasers and Applications in Atmospheric Sensing, Alan Fried, Editor,
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- Reliability, Stability – Diode lasers, as well as all of the electronic components, are all solid state devices with a proven record of long term stability and lifetime. As mentioned above, the approach toward absorption overcomes any degradations in time of laser power on the detectors. Optical absorption methods do not exhibit any of the hysteresis effects commonly found in solid state sensors. There is no need for any routine maintenance since the sensor runs unattended and uses no consumables.
- Selectivity – Optical absorption spectroscopy based on individual lines of gases is extremely selective; with properly chosen lines, only the desired gas contributes to the measurement signal, even in very complex mixtures.
- Size and weight– Using digital signal processors (DSP) in surface mount configurations, the entire sensor package is extremely compact. The major size factor is the required optical absorption path length, which depends on the gases and sensitivity levels required. Packaging is flexible and the sensor could be deployed as a portable, battery-powered handheld unit as well as in stationary locations.
- Electrical Power – In typical diode laser gas sensor systems, the largest demand for power arises from the thermoelectric coolers (TEC; drawing up to 5 Watts) and the DFB laser (0.25 W). The use of vertical cavity lasers (VCSELs), which draw only about 5-10 mW is a significant improvement. The custom VCSEL lasers we use are mounted directly onto a miniature TEC inside the laser housing, reducing its load to below 300 mW. In addition, conventional control and analysis electronics (computers, and particularly analog I/O chips) draw many watts of power. DSP chips and the I/O interfaces, developed for use in cell phones and other portable devices, run at lower voltages and much lower currents so that our complete two-laser system, based on these components, will draw only about 3 W.
- Safety – Solid state sensors are safe, contain no hazardous chemicals and use low voltages at low currents. The laser output powers are very low and eye-safe.

Table I - Multigas Sensor Specification Goals

Property	Specification
Number of lasers	2
Number of gases	2 - 3
Size	3½″ × 1½″ × 1″
Weight (oz.)	~ 6
Power (W)	3
Gas sensitivities	O_2 0.1% CO_2 10 ppm
Accuracy	2% of reading
Precision	< 1% of reading

2. EXPERIMENTAL

The multigas sensor, shown in Fig.1, contains a detachable optical unit that can be mounted onto a custom circuit board containing the laser current and temperature controllers, preamplifiers, diagnostic LEDs. The circuit board plugs into a commercial DSP controller (Innovative Integrations SBC6701 with dual OMNIBUS A4D4 I/O cards). The entire assembly is 2.5″× 4″ × 6″ in size, weighs 2.91kg and uses 10 W of power.

The optical head comprises a copper block that holds both lasers and silicon and extended-InGaAs photodiodes for detection of O_2 and CO_2, respectively. Both laser outputs are focused by aspheric lenses onto flat mirrors which point the beams into the detectors. The total optical open air paths are 17 cm. A pressure and ambient temperature sensor also mount onto this unit.

Both laser TEC's are driven by Wavelengths Electronics WTC3243 ultrastable thermoelectric controllers. The DFB laser is controlled by a Wavelengths Electronics WLD3343 laser driver. Since the VCSEL draws only a few mA, a simple op amp is used to control its injection current. A major feature of the sensor is that it is comprised entirely of solid state components and is designed to be totally autonomous. The Texas Instruments TMS320C6701 DSP chip runs at 160 MHz with 1 GFLOP and 64 kB of on-chip memory. The program is downloaded through a JTAG interface to 128 kB of flash ROM. Upon powering up the board, the program automatically boots and runs. Sixteen MB of SDRAM are available for memory usage and data storage. A pair of 16-bit, 200 kHz independent A/D and D/A chips are used to ramp and modulate

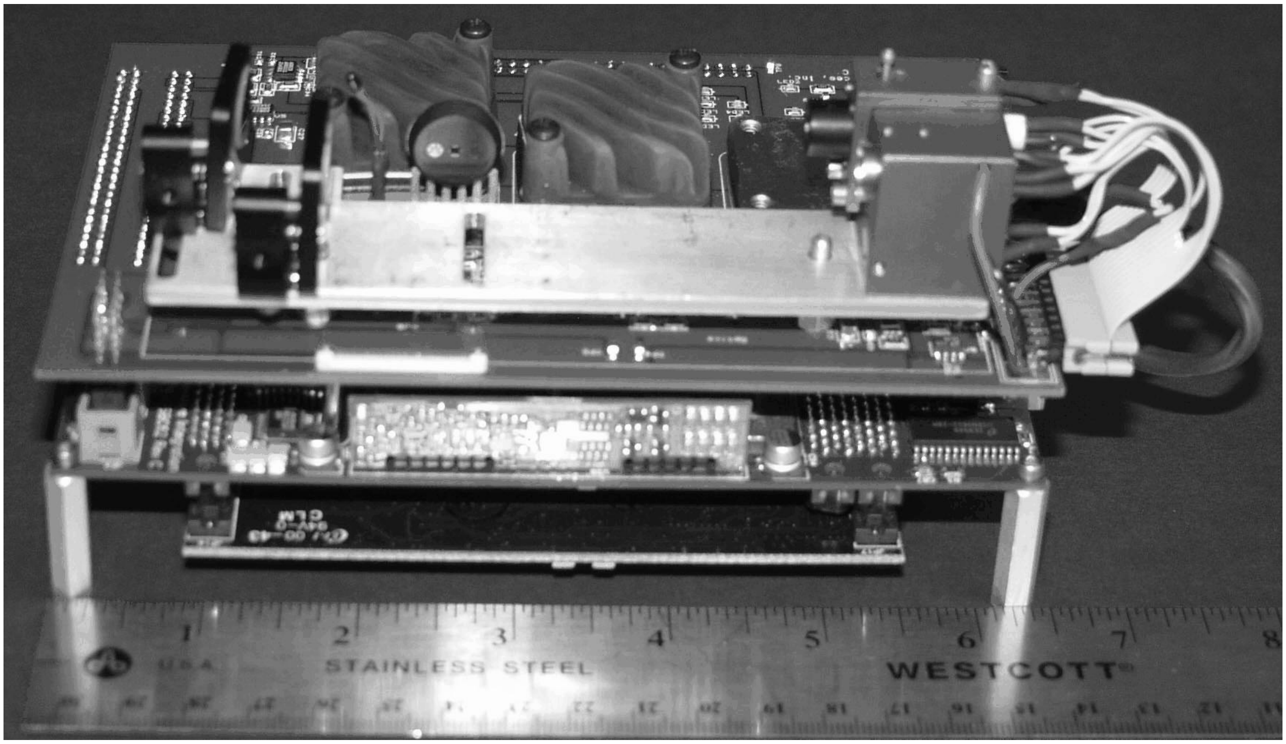


Figure 1 - Photograph of multigas sensor.

the lasers and collect the photodiode signals. Slower A/D's are used to read temperatures and pressure. An RS-232 serial port communicates with a 4 × 20 character fluorescent display that reports concentrations, ambient conditions and errors. Two additional analogs ports are used to relay the measured gas concentrations to a computer for recording data over longer periods of time.

Gas absorbances are measured using 2*f* wavelength modulation spectroscopy.[1; 2] The modulation frequency is 17.5 kHz and the linear ramp with superimposed modulation is clocked by the DSP board at 200 kHz. The lasers are scanned across approximately 1 cm^{-1} and 20 spectra (normalized to the total laser intensity) are recorded and averaged per second. These data are then fit to a theoretical reference spectrum determined using the known modulation depth, calibrated wavelength scale, and measured temperature and pressure. In these scans, the wavelength scale is non-linear in injection current and a solid etalon is used to determine the correspondence between wavelength and current. The fitting algorithm uses singular value decomposition (SVD)[3] of a design matrix comprising the reference line shape, its derivative (used to precisely locate the peak for line-locking[4]) and a polynomial set of background terms. Despite the computational intensity required for this analysis, it is readily accomplished with the DSP chip.

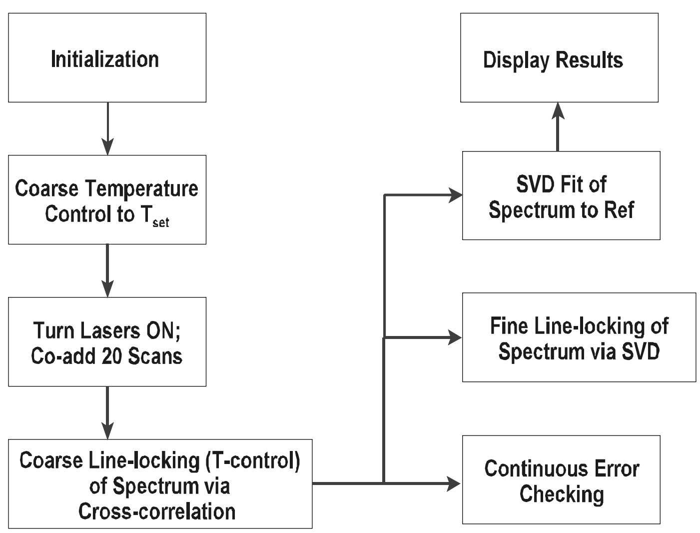


Figure 2 - Control and analysis flow chart.

The sequence of operation is shown in Fig. 2. Initial laser temperatures are set using the thermistors mounted near the lasers, but once the lasers have approximately reached operating temperature, they are turned on and the peaks of spectra are used for line-locking to the center of the scan by a feedback loop to the control temperature.

For this work, the RR(7,7) line in the $v' = 0 \leftarrow v'' = 0$ transition of the $b\,^1\Sigma \leftarrow X\,^3\Sigma$ band at 13098.8 cm^{-1} is used for O_2 and the R18 line in the $\nu_1+2\nu_2+\nu_3$ band at 4991.26 cm^{-1} for CO_2. The HITRAN database[5] provides all spectral parameters for both gases, except for broadening coefficients for O_2 which are obtained from Ritter.[6]

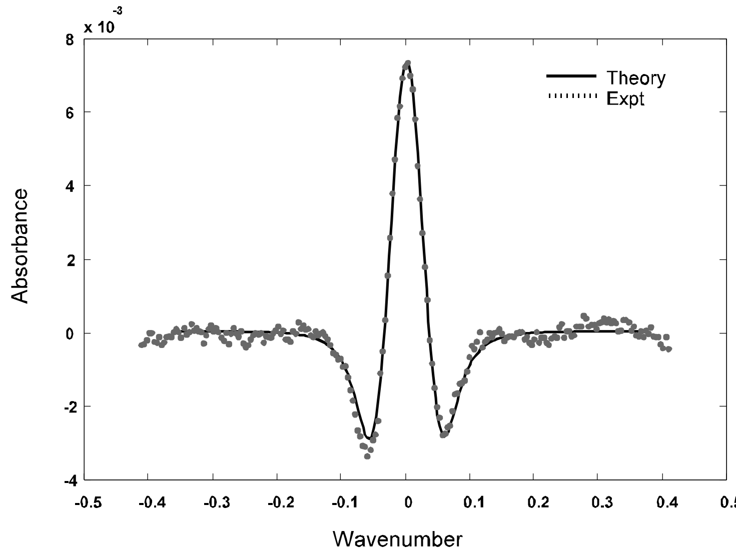


Figure 3 - Theoretical and experiment 2f line shapes.

3. RESULTS

A series of measurements were performed to quantify the operating characteristics of the multigas sensor. These include accuracy, precision, linearity and time response. Figure 3 illustrates a typically measured and best fit 2*f* line shape for ambient O_2 (20.95%). Despite this large mole fraction, its very weak line strength limits the absorbance to ~1%. In contrast, CO_2 has a strength about 150 time larger, thus the better sensitivity at lower concentrations.

Figure 4 is a plot of measured mole fraction of oxygen ranging from 2 to 25%. The results indicate that, as expected, the optical system responds linearly ($r^2 = 0.998$).

The system has been run for up to 3 days unattended, logging the concentration of oxygen and carbon dioxide with a 1 Hz bandwidth. During this period, line-locking was never lost. For two days, the system ran in ambient air, and while small fluctuations are expected for carbon dioxide, since people breathing near the system can be detected, there were additional variations that still need to be explained. However, these changes appear to be correlated for both gases and we suspect that the pressure gauge (whose output is proportional to the supply voltage) may be the cause. The next version of this instrument will use a voltage reference to power the pressure gauge.

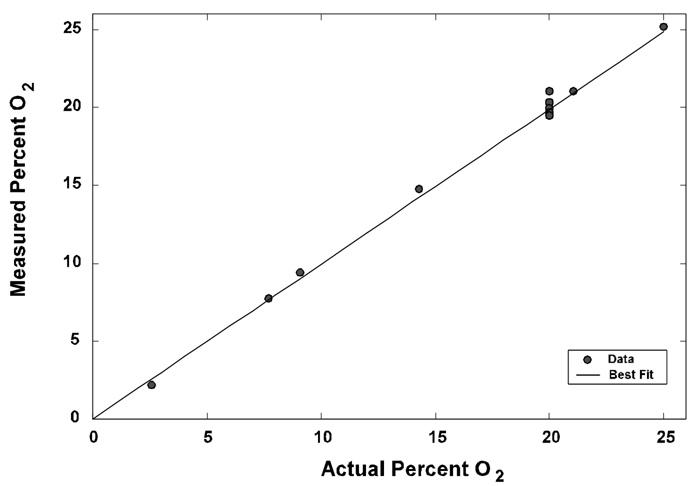
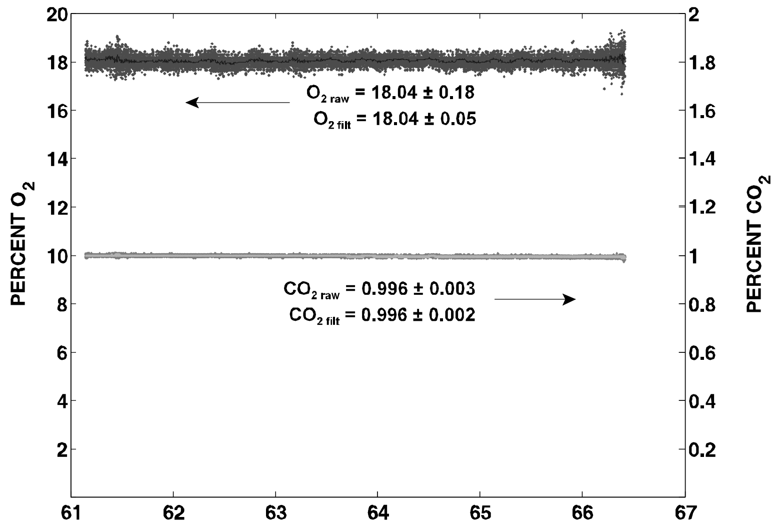


Figure 4 - Linearity measurement for O_2 detection.

In Fig. 5, we show a five and one-half hour period where a calibrated mixture of 0.96% CO_2 in dry air was constantly flowed over the sensor housed in a plastic enclosure. This test evaluates the inherent system stability. As seen in the figure, very flat, noise-free results are observed, with one standard deviation for the entire period equal to about 1% of the concentration for O_2 and 0.3% for CO_2.

To improve noise rejection, yet retain good overall time response, a Kalman-Bucy adaptive filter[7] was incorporated into the analysis program. The attractive feature of this algorithm is that it requires very little memory storage and is robust to real-time changes in the data. As seen in Fig. 5, the filter provides substantial smoothing. For the calibrated gas mixture, the stability of the instrument is better than 0.4 % for oxygen (peak absorbance of $\sim 4 \times 10^{-3}$) and 0.2 % for CO_2 (peak absorbance $\sim 1 \times 10^{-2}$).

In order to measure the ultimate instrument precision, which would be limited by drift at longer integration times, an Allan variance for 1% CO_2 in air was computed from the long term measurements, as shown in Fig. 6. As expected, the standard deviation decreases as the square root of time until overcome by instrumental drift at about 100 sec integration time. At this point, the precision is $\sim 3 \times 10^{-4}$ of the signal.



4. CONCLUSIONS

A multigas sensor has been demonstrated to meet many of the stringent requirements for use in space-borne vehicles. It can run unattended for extended periods of time and has a complete set of on-board diagnostics. Gas concentrations are reported in real time and its size, weight, and power are suitable for operation as a sensor for monitoring plant growth or other applications important to space flight. Precision, linearity and accuracy are quite good, and CO_2 measurements have an excellent dynamic range.

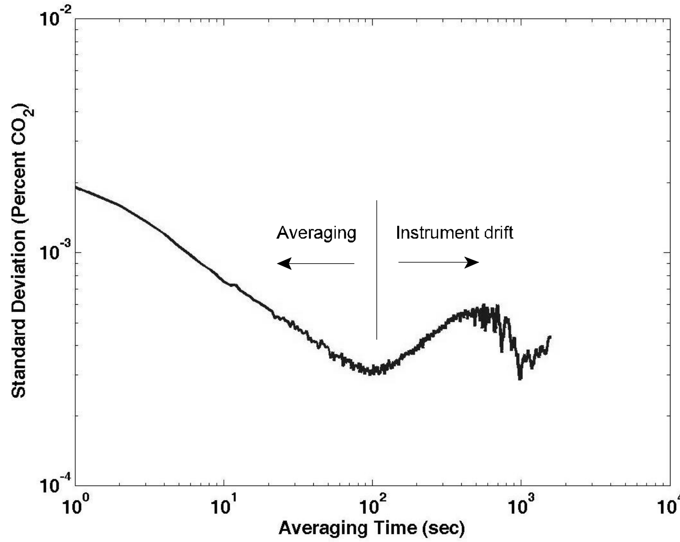


Figure 6 - Allan variance for 1% CO_2 in dry air.

This sensor is under continuing development and the next version will use a customized DSP board (with a more power efficient TMS320C6711 chip). This, along with the use of low power I/O circuitry and improvements to the laser head, will result in a system about half the size of the current device, with an estimated power usage of about 3W. These characteristics make this system attractive for battery-powered, hand-held uses. Additionally, we will study the possibility of detecting water vapor with the 2000 nm laser, as it has weak absorption features adjacent to other CO_2 lines accessible in this wavelength region.

ACKNOWLEDGMENTS

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REFERENCES

1. J. A. Silver, "Frequency-modulation spectroscopy for trace species detection: theory and comparison among experimental methods," *Appl. Opt.* **31**, 707-717, 1992.
2. D. S. Bomse, A. C. Stanton and J. A. Silver, "Frequency-modulation spectroscopy for trace species detection: comparison of experimental methods using a lead-salt diode laser," *Appl. Opt.* **31**, 718-731, 1992.
3. W. H. Press, *et al.*, *Numerical Recipes in C: The Art of Scientific Computing.* Cambridge, Cambridge University Press, 1995.
4. D. C. Hovde, *et al.*, "Wavelength modulation hygrometer for ultrasensitive detection of water vapor in semiconductor gases.," *Appl. Optics* **40**, 829-839, 2000.
5. L. S. Rothman, *et al.*, "The HITRAN molecular spectroscopic database and HAWKS (HITRAN atmospheric workstation): 1996 edition," *J. Quant. Spectrosc. Radiat. Transfer* **48**, 665-710, 1998.
6. K. J. Ritter and T. D. Wilkerson, "High-Resolution Spectroscopy of the Oxygen A Band," *J. Mol. Spectrosc.* **121**, 1-19, 1987.
7. R. E. Warren, "Adaptive Kalman-Bucy filter for differential absorption lidar time series data," *Appl. Opt.* **26**, 4755-4760, 1987.