The MVACS tunable diode laser spectrometers

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Abstract. Two independent tunable diode laser spectrometers are resident aboard the Mars Polar Lander as part of the Mars Volatiles and Climate Surveyor payload. One spectrometer is located on the meteorological mast for measurements of H₂O and CO₂ in the free atmosphere, and the other serves as the H₂O and CO₂ analyzer for the Thermal and Evolved Gas Analyzer. Water vapor is measured using a tunable diode laser operating at 1.37 μ m, while CO₂ is measured using a second laser operating near 2.05 μ m. The 2.05 μ m laser also has isotopic analysis capability. In addition to the major CO₂ isotopomer (¹²C¹⁶O¹⁶O), analyses of ¹³C¹⁶O¹⁶O and ¹²C¹⁸O¹⁶O in the atmosphere and in the Thermal and Evolved Gas Analyzer are possible under certain conditions. The spectrometers were designed and built at the Jet Propulsion Laboratory and have their heritage in a series of tunable diode laser spectrometers developed for Earth atmospheric studies using high-altitude aircraft and balloon platforms. The 1.37 μ m diode laser on the meteorological mast will provide the first in situ measurements of water vapor in the Martian boundary layer, with a detection sensitivity an order of magnitude greater than the water vapor abundances inferred from the remote-sensing observations by the Viking Orbiters.

1. Introduction

Tunable diode lasers (TDLs) have been used in highresolution spectroscopic studies of gases since the 1970s [e.g., Mantz and Eng, 1978]. Their extensive wavelength coverage (0.5–30 μ m), rapid and continuous tunability, and narrow spectral linewidth make them ideal as light sources in gas-sensing spectrometers. Lead-salt TDLs cover the wavelength region from 3.2 μ m to beyond 30 μ m but require cooling to temperatures typically below 120 K, which prohibits their use on an extended planetary mission such as the Mars Polar Lander (MPL). TDLs that operate continuous wave at wavelengths in the 0.6–2.1 μ m region at much higher temperatures (up to 50°C) are available as a result of extensive development by the optical communications industry. That industry requires single-frequency lasers operating at the near-infrared wavelengths of 1.3 and 1.55 μ m, where optical fiber attenuation coefficients are at a minimum. Early work at the Jet Propulsion Laboratory (JPL) [Forouhar et al., 1992] extended the wavelength range of single-frequency, high-temperature (300 K) devices to near 2.1 μ m, which enables a wide range of gases to be monitored using overtone or combination bands present in the near-infrared region.

H₂O and CO₂ both have relatively strong absorption bands in the 1-2 μ m region. The $\nu_1 + \nu_3$ combination band of H₂O is centered near 1.38 μ m, while three bands of CO₂ and its isotopomers occur in the 2 μ m spectral region. Isotopic bands

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Paper number 1999JE001146. 0148-0227/01/1999JE001146\$09.00 of these molecules will be shifted in wavelength relative to the primary isotope. A careful analysis of the spectra of H₂O and CO₂ was undertaken to select the optimum measurement regions for the Mars Volatiles and Climate Surveyor (MVACS) TDL spectrometers. One TDL spectrometer is located on the meteorological (MET) mast, and the other is part of the Thermal and Evolved Gas Analyzer (TEGA). For MET the goal was to select a CO₂ spectral region containing as many isotopic lines as possible while simultaneously avoiding the very strongest main isotope lines, which would be too optically deep in the Martian 95% CO₂ atmosphere. For TEGA the emphasis was placed on obtaining a low detection threshold for the main CO₂ isotopomer while maintaining the ability to monitor the carbon-13 and oxygen-18 isotopomers. Although HDO measurements are technically possible if the water vapor abundance is sufficiently large and long-term spectrum averages are performed, detection of HDO is marginal owing to the extremely weak absorption levels expected in the 1.37 μ m region.

Other papers in this special issue address the scientific rationale for the measurements of water vapor and carbon dioxide, and isotopic composition on Mars, and provide detailed descriptions of the MET and TEGA instruments [Boynton et al., this issue; D. Crisp et al., manuscript in preparation, 2001]. In this paper the technical details of the two MVACS TDL spectrometers are presented, along with brief descriptions of the calibration and data-processing methods, which are described in detail elsewhere [May and Webster, 1993; May, 1998].

2. Heritage

The TDL sensors developed for MVACS have their heritage in a series of TDL spectrometers developed at JPL beginning in the early 1980s. At that time, diode lasers required cooling to temperatures in the 20–60 K range using liquid helium dewars, and field instrumentation was necessarily physically large and expensive. In 1985 the first mid-IR (3–10 μ m) TDLs became available; they operated at 77 K, and slightly above, enabling a significant reduction in instrument size as liquid

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nitrogen could replace liquid helium as the cryogen in the laser dewars. A balloon-borne, multilaser TDL spectrometer (BLISS) was flown successfully 12 times between 1982 and 1992 [Webster and May, 1987; Webster et al., 1990a] and made measurements of NO, NO₂, HNO₃, O₃, CH₄, N₂O, HCl, H₂O, HDO, and CO₂ in the Earth's atmosphere. Both liquid helium and liquid nitrogen dewars were utilized on BLISS, and the instrument package had a mass of nearly 1000 kg.

The success of the BLISS instrument led to the development of the aircraft laser infrared absorption spectrometer ALIAS, a much smaller, four-channel TDL spectrometer for the NASA ER-2 aircraft [Webster et al., 1994] which used only lasers that could operate at temperatures above 77 K. This instrument and a two-channel version developed for a balloon platform (ALIAS-II [Scott et al., 1999]) are both currently operational and participating in NASA field campaigns. Each houses the TDLs in a liquid nitrogen dewar with a typical operational time between cryogen refilling of >12 hours (30 hours nonoperational). ALIAS-II has a mass of 28 kg; although small relative to prior configurations, it is still a research-grade field spectrometer requiring daily cryogen replenishment. In 1990 the probe infrared laser spectrometer (PIRLS) instrument was proposed for the NASA Cassini mission by Webster et al. [1990b]. This instrument design utilized a novel Joule-Thomson cooler developed at JPL to cool lead-salt TDLs to near their nominal 80 K operating temperature and was also equipped with a particle size spectrometer. It was the first comprehensive effort at designing and breadboarding a spacequalifiable TDL spectrometer at JPL. Total instrument mass for PIRLS was \sim 5 kg.

At present, diode lasers operating continuous wave at wavelengths longer than 2.1 μ m must be cryogenically cooled, and many gases of interest can be monitored only at low levels (parts per billion and below) using mid-IR lasers which can access the fundamental vibration bands. However, water vapor has a relatively strong absorption band centered at 1.38 μ m which is accessible using TDLs that do not require cryogenic cooling. CO₂ and several of its isotopes can be measured at 2.05 μ m using similar lasers. In 1992, near-IR (1-2 μ m) diode lasers were developed at JPL and were optimized during the next 3 years for use in a new class of TDL spectrometer. These devices produced single-frequency output as a result of the distributed feedback (DFB) structure [Forouhar et al., 1993] and provided several milliwatts of continuously tunable output. In 1996 the first TDL-based JPL aircraft instrument for measurements of water vapor from the NASA high-altitude ER-2 research aircraft was flown [May, 1998], and in 1998 a version for the NASA DC-8 was deployed to make measurements in thunderstorms and hurricanes as part of the third Convection and Moisture Experiment (CAMEX-3). These near-IR aircraft instruments formed the basis for the design of the MVACS spectrometers, which incorporate many of the same basic design features.

Substantial reductions in mass, volume, and power consumption were necessary for integration into the MVACS payload. Initially, only measurements of water vapor in the free atmosphere were to be undertaken. As the instrument design phase progressed, a second laser was added with the goal of analyzing the abundances of isotopic CO_2 in the atmosphere, and eventually a dual laser system was also selected as the evolved gas analyzer for the TEGA. Volume and power constraints led to significant design compromises that resulted in reduced sensitivity for the MVACS TDL spectrometers in comparison to those developed at JPL for aircraft and balloon platforms. However, the primary science goals of H_2O and CO_2 detection in the Mars atmosphere, and in evolved gas samples, can be met with the flight hardware. In the following sections the instrument design details are given along with specifications and expected performance for the MET and TEGA TDL spectrometers.

3. Instrument Descriptions

The MET and TEGA TDL spectrometers share common designs for several subsystems. Among these are the control and signal-processing electronics (jumpered for slightly different operation on the two systems), the laser and detector optical mounting assemblies, and multipass (Herriott) absorption cells used to increase the optical absorption path length. Differences between the MET and TEGA systems include the Herriott cell mirror sizes and focal lengths, minor thermal control details, and the exact laser wavelengths used to monitor the chosen H_2O and CO_2 rovibrational lines. Table 1 summarizes the spectrometer specifications. The minimum detectable absorption levels listed are direct measurements from recorded spectra.

3.1. Lasers

Distributed feedback (DFB) lasers operating at 1.37 and 2.05 μ m [Forouhar et al., 1992, 1993] were fabricated and flight-qualified at JPL for the MVACS TDL spectrometers. These devices operate on a single longitudinal mode with a side mode suppression of >30 dbar, so spectral interference from minor modes is negligible. The laser chips are mounted in 5.6 mm cylindrical "TO" packages and hermetically sealed in the packages with welded endcaps containing antireflection (AR) coated windows. Output power is in the 5–8 mW range for the 1.37 μ m lasers and 2–3 mW for the 2.05 μ m lasers. Continuous tuning ranges exceeded 2 cm⁻¹ for all devices.

3.2. Electronics

TDL control and signal-processing electronics are contained on a single, six-layer circuit board measuring 8.4×19.1 cm, which is mounted in the payload electronics box (PEB). The circuit consists of two functional sections for each laser/ detector channel that are associated with control of the laser current and detector signal processing. A block diagram of the TDL circuitry is shown in Figure 1. Spectra are recorded by holding the laser temperature fixed and changing the wavelength by varying the injection current. The laser current is swept repetitively over a range of a few tens of milliamperes, which corresponds to a spectral region of about 2 cm^{-1} . A novel design for controlling the laser scan waveform was developed for MVACS and is described in detail by Woodward and May [1999]. A programmable ROM holds two laser scan waveforms that are continuously "played out" to the laser drive circuitry via logic that cycles through the ROM addresses and delivers a programmed laser current value to the appropriate laser. A small-amplitude (~0.5 mA peak) sine wave is superimposed onto the base laser scan ramp to enable second harmonic (2f) detection. Both the ramp and sine wave amplitudes are programmable, as are the ramp beginning and end points which define the spectral scan region. For the MVACS TDL spectrometers the laser scan period is fixed at 2.79 s, limited by the rate at which data could be transmitted across the 9600

Parameter	MET	TEGA
Mass, kg, excluding electronics	0.5	0.44
Power consumption, W, maximum	4.3	4.5
Optical path length, cm	1055.6	100.8
Mirror separation, cm	27.78	5.60
Mirror diameter, cm	3.40	2.54
Mirror center thickness, cm	0.5	0.4
Mirror substrate material	Zerodur	Zerodur
Mirror optical coating	Cr-Au, Al ₂ O ₃ overcoat	Cr-Au, Al ₂ O ₃ overcoat
Number of beam passes	38	18
Inner coupling hole radius, cm	0.90	0.47
Outer coupling hole radius, cm	1.30	0.87
Detector (active area diameter)	InGaAs (1 mm)	InGaAs (1 mm)
H ₂ O laser set point, °C	22.8	2.9
CO_2 laser set point, °C	17.9	-3.5
Beam injection angle, deg		
Inner hole	1.703	3.974
Outer hole	2.460	7.356
Nominal beam diameter (cm), all lasers	0.25	0.25
H_2O spectral region, cm ⁻¹	7297.97300.4	7306.0-7307.5
CO_2 spectral region, cm ⁻¹	4885.0-4886.9	4876.7-4878.6
Minimum detectable absorption level	4×10^{-4}	8×10^{-4}
H_2O minimum detectable abundance, cm ⁻³	$5.6 imes 10^{11}$	$1.0 imes 10^{13}$
\tilde{CO}_2 minimum detectable abundance, cm ⁻³	$4.2 imes 10^{14}$	$7.2 imes 10^{14}$

Table 1. Tunable Diode Laser Spectrometer Specifications

baud serial link to the lander computer. The laser modulation frequency is 2.93 KHz (2f detection frequency 5.86 KHz).

Detector signals are provided as inputs and are processed using standard second harmonic detection techniques [Webster et al., 1988; May and Webster, 1993; May, 1998]. Briefly, both the dc and ac components of the detector signal are extracted and downlinked for processing. The dc component represents the laser power and is required for normalization of the ac signal. The ac component is the second harmonic spectrum obtained by demodulation of the detector signal at 5.86 KHz (twice the laser modulation frequency). Figure 2 shows examples of dc and 2f spectra recorded by the TEGA TDL for a pure CO₂ sample. The laser power increases with injection current, which produces the sloping baseline in the dc spectrum. Since the 2f signal amplitudes are proportional to the received laser power at the detector, the dc spectrum must be used for normalization before the 2f signals can be used for quantitative determination of gas concentration. No spectrum processing is performed by the lander computer.

3.3. Optics

Both the MET and TEGA spectrometers utilize multipass "Herriott" cells [Herriott et al., 1964; Altmann et al., 1981]. These configurations produce a 1.0 m optical absorption path for the TEGA spectrometer and a 10.6 m absorption path for the MET spectrometer. For each Herriott cell the laser beams are coupled into the system via holes in one mirror (the "coupling" mirror) that lie on different radii so that two nonoverlapping spot patterns are formed on the mirror pairs. The beams exit the system through the input coupling holes and impinge upon detectors which are mounted on the same thermal plate as the lasers. For each system the two laser beams make nearly circular spot patterns on the Herriott cell mirrors with radii defined by the coupling hole positions. The two mirrors in a Herriott cell have the same radius of curvature. Zerodur was chosen as the mirror substrate material for both the MET and TEGA systems, with Cr-Au as the reflective coating. An Al₂O₃ overcoat protects the Au surfaces. This

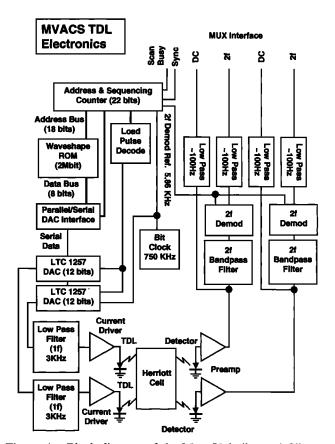


Figure 1. Block diagram of the Mars Volatiles and Climate Surveyor (MVACS) tunable diode laser (TDL) control and signal-processing electronics. Laser current scan waveforms are stored in the waveshape ROM and continuously played out to the laser current driver circuitry to sweep the lasers over the designated wavenumber range. The dc component of the detector signal is amplified and low-pass-filtered and supplied as an analog output signal. The ac component at 5.86 KHz is the second harmonic (2f) spectrum and is extracted using a bandpass filter, a synchronous demodulator, and a low-pass filter.

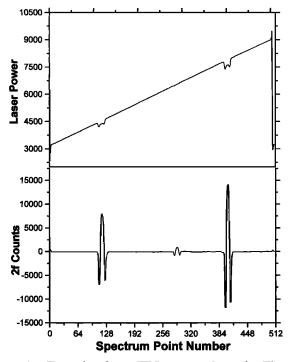


Figure 2. Example of raw TDL spectra from the Thermal and Evolved Gas Analyzer (TEGA) spectrometer for a pure CO_2 gas sample at approximately 9 mbar pressure and 300 K temperature. The laser power (shown in analog to digital (A/D) converter counts) increases with laser injection current, and the modulated CO_2 lines are visible in the upper spectrum. The lower spectrum is the 2f spectrum, which must be normalized to the laser power spectrum for quantitative analysis. For this process a polynomial baseline is fit to the laser power spectrum and the value at the 2f line center peaks used for normalization of the 2f signal amplitudes.

coating was found to perform extremely well with the external optics flown on the NASA ER-2, WB57F, and DC-8 aircraft experiments, which were subjected to $>200 \text{ m s}^{-1}$ airflow continuously during flights. No significant reduction in mirror reflectivity was observed after more than 500 flight hours. Thus, for the MET system we do not expect mirror damage from dust or aerosol impact for typical wind conditions on Mars.

Figure 3 shows a single laser/detector assembly (for the TEGA 2.05 μ m laser) which illustrates the basic design employed for laser and detector mounting for all four MVACS laser/detector heads. A single aspheric lens is used to collect and collimate the laser output beam. This arrangement produces a collimated ellipse with a major/minor axis ratio of approximately 3. The lens is positioned to achieve a beam focus that is slightly beyond the midpoint between the Herriott cell mirrors. This results in a beam spot size at the detector that is optimum for the 1 mm detector area without the need for a second collecting/focusing lens at the detector.

Two angled aluminum (Al) mounts hold the laser packages at the appropriate Herriott cell injection angles. The laser collimating lens is a 4.5 mm diameter asphere with 4.5 mm focal length and is mounted to the same Al piece that holds the laser package. Each detector is a 1 mm diameter InGaAs photodiode operated with zero bias voltage. Extended-range InGaAs detectors are used for the 2.05 μ m lasers. The laser/ detector separation is a function of distance from the Herriott cell coupling mirror as determined by the composite angle between the entrance and exit beams. A 6.6×6.6 mm, 1.72 W thermoelectric cooler (TEC) is sandwiched between the Al laser mount and a second Al bracket which serves as both the "sink" for the TEC and the supporting mount for the laser/ detector assembly. Each TEC operates as a cooler or a heater, as required, but will function primarily as a heater at Mars because the laser set points (near 0°C for TEGA and near 20°C for MET) are above the expected ambients during most of the mission. Both the laser and detector temperatures are held constant within ±0.01°C using hybrid controller circuits provided by Hytek Microsystems Inc. (Carson City, Nevada). These controllers were configured for true proportionalintegral-derivative (PID) operation to minimize overshoot on power up. To further improve laser temperature setpoint stability against excursions of Mars ambient, MET TEC controller circuitry includes provision for electronic compensation of the effects of finite thermal conductivity of the Al mount block. This novel arrangement dynamically adjusts controller setpoint as a function of TEC power input to anticipate and partially cancel temperature control errors resulting from thermal gradients within the laser mount assembly.

3.4. MET

The MET spectrometer consists of an open-path Herriott cell mounted on the MET mast and two diode lasers for measurements of atmospheric H_2O and isotopic CO_2 . Figure 4 shows the layout on the MET mast. The optical absorption pathlength for both MET TDL channels is 10.6 m. The multipass mirrors are mounted in fixed locations on the mast and exposed to the free atmosphere. Temperature and pressure data, required for TDL spectrum processing, are supplied by independent sensors whose details are described by D. Crisp et al. (manuscript in preparation, 2001). Owing to sequencing and data acquisition constraints, spectra of H_2O and CO_2 are not acquired simultaneously but are recorded alternately with only one of the two lasers operating at any given time.

In Figure 5, example spectra are shown from single laboratory scans of each MET laser (2.79 s acquisition time). These spectra were recorded with the lasers mounted in custom laboratory test fixtures which allowed the laser operating temperature and current to be adjusted easily. In addition, the necessary alignment adjustments were available to minimize optical fringing in the spectra. In the flight systems, there was insufficient movement in the collimating lens position in the plane perpendicular to the optic axis of the lens to achieve optimum alignment. Therefore optical fringing levels in the spectra are significantly higher than they would be for a properly aligned system and are the limiting noise factor by a full order of magnitude. Baseline center absorption levels are in the 5 \times 10⁻⁴ range, which can be translated into equivalent minimum detectable number densities using Beer's law. The results are listed in Table 1. The effects of optical fringing can be reduced somewhat by fitting and analysis procedures, as well as spectrum averaging. Figure 6 shows an example of fringe reduction for a single MET CO₂ spectrum. Such techniques will be required to extract maximum information from the MVACS TDL spectrometers owing to the excessive amplitude of the optical fringes in the spectra. For comparison, the Viking MAWD instruments [Farmer and Doms, 1979] measured minimum water vapor abundances of approximately one precipitable micron, which, if uniformly mixed with pressure, would yield surface water vapor concentrations of the order of $3.0 \times 10^{12} \text{ cm}^{-3}$.

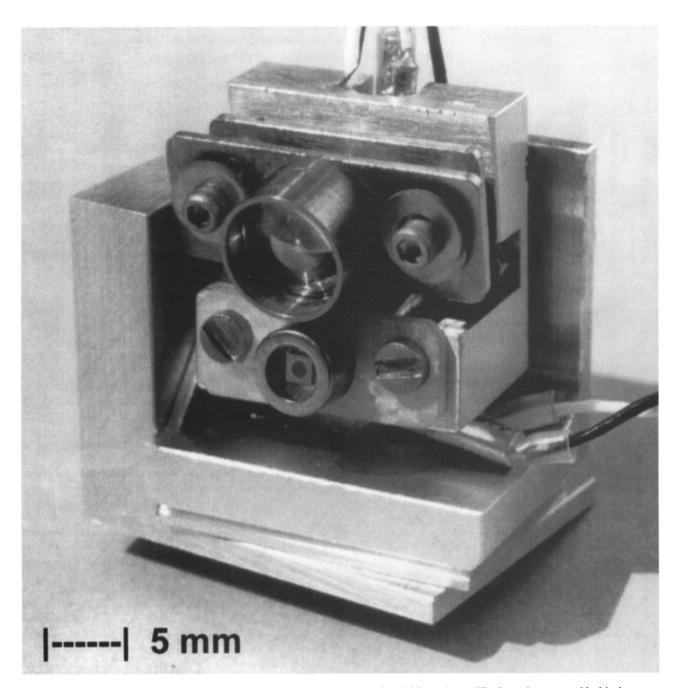


Figure 3. Photograph of a laser/detector package for the TEGA 2.05 μ m laser. The laser is mounted behind the collimating lens, which is visible as the upper circular optic. The detector is mounted directly below the laser and is not equipped with a collimating lens. Appropriate injection angles for the Herriott cells were machined into the mounting pieces, eliminating the need for external beam-steering mirrors.

3.5. TEGA

The TEGA spectrometer is a closed-path system where evolved gases are brought into the Herriott absorption cell via heated transfer lines and a stream of N_2 carrier gas. Details of the TEGA instrument are given by *Boynton et al.* [this issue]. The multipass mirrors are mounted within an insulated Al tube. Figure 7 shows the layout of the TEGA TDL spectrometer and indicates the positioning of the laser/detector assemblies with respect to the Herriott cell mirrors. Note that a portion of the optical path includes the area within the optical head between the laser and the Herriott cell coupling mirror and the area between this mirror and the detector. Fused silica windows attached to the back of the coupling mirror isolate the internal Herriott cell volume (and optical path length) from the optical head, but the optical head is not purged and will contain ambient mars atmosphere. Absorption within this portion of the optical path will be taken into account by recording spectra while pure N_2 purge gas is flowing through the Herriott cell and subtracting the resulting spectrum from the spectra recorded during the subsequent heated sample run.

Example spectra recorded with the flight unit are shown in Figure 8. Unlike the MET system, both lasers are operated

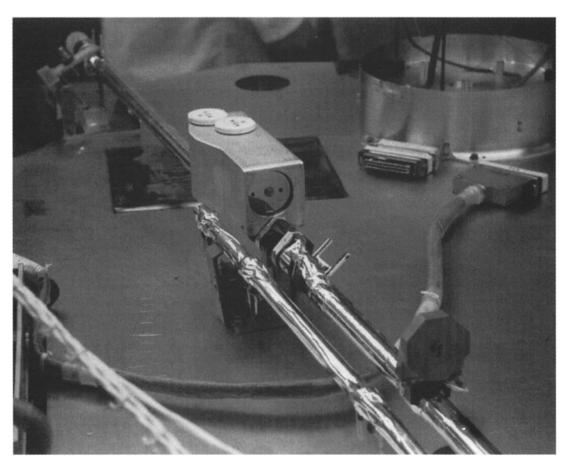


Figure 4. Photograph of the meteorological (MET) TDL spectrometer as mounted on the MET mast. The optical heads are contained in an Al enclosure shown toward the rear of the photograph with the two radiator disks on top. The face of the Herriott cell coupling mirror can be seen here, with the opposing Herriott cell mirror mounted in an Al mount located ~ 28 cm away (Table 1).

during sample runs for the TEGA so that spectra of H_2O and CO_2 can be acquired simultaneously. As with the MET spectrometer, optical fringes limit the sensitivity owing to absence of necessary optical adjustments for the TDL collimating lens. Conventionally, IR spectra are displayed in wavenumber (cm⁻¹) units, with wavenumber increasing from left to right as shown. Because the near-IR diode lasers tune such that wavenumber decreases (wavelength increases) with increasing current, the spectra shown in Figure 8 (and Figure 5) are reversed in comparison to the raw spectral data that are downlinked (e.g., compare the peak positions in Figures 2 and 8).

4. Calibration and Data Analysis

Second harmonic detection is implemented for the MVACS spectrometers. Details of this detection technique, and data interpretation methods, are given by *Webster et al.* [1988], *May and Webster* [1993], and *May* [1998]. Briefly, a constant-period sawtooth current ramp is applied to the TDL to scan the output wavelength over the desired spectral interval (typically $1-3 \text{ cm}^{-1}$). A small-amplitude sinusoidal waveform at frequency f is added to the ramp, and the detector signal is demodulated at 2f to produce the second harmonic spectrum. The amplitude of the sinusoidal modulation is adjusted to produce the optimum 2f spectrum based on the conditions of the measurement. Since the molecular line shape varies with

pressure and temperature, some care is required in choosing the optimum modulation amplitude if its value is not continuously updated by the software on the basis of current pressure and temperature measurements. For MVACS the modulation amplitude is held fixed for all lasers at values optimum for 7 mbar pressure (MET) and 15 mbar (TEGA) because the modulation amplitude is programmed into the waveform ROM and cannot be changed during operations at Mars.

Molecular number densities are extracted from the observed second harmonic signal amplitudes using the Beer-Lambert law and appropriate analysis of the second harmonic line shapes. Full details are given by May [1998] and are therefore not repeated here. Calibration of the 2f signal chain is accomplished by comparing the direct absorption spectrum to the corresponding 2f spectrum and formulating a "response" number R for each signal chain. Details are described by May and Webster [1993]. Figure 9 shows a modulated direct transmission spectrum (dc spectrum) for a pure CO₂ sample. A modulated direct transmission spectrum will accompany each MVACS 2f spectrum, and when the concentration of the target gas is sufficient to observe the spectral line in the direct transmission spectrum, it will be possible to confirm the R number values from the actual Mars spectra. The direct transmission spectral line is split from the wavelength modulation, which places the laser wavelength off of the line at the extremes of the cosine

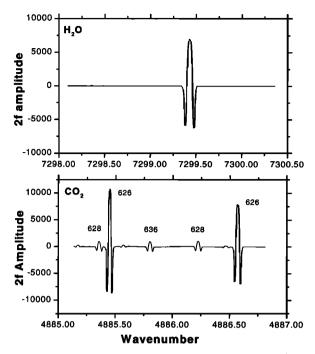


Figure 5. Spectral regions chosen for monitoring (top) H_2O and (bottom) CO_2 for the MET TDL spectrometer. The numeric labels in the CO_2 spectrum identify the isotopomers ($626 = {}^{12}C^{16}O^{16}O$, $636 = {}^{13}C^{16}O^{16}O$, $628 = {}^{12}C^{16}O^{18}O$). Signal amplitudes are in counts from the A/D converter.

modulation function. The dashed line in the modulated direct transmission spectrum is a synthetic best fit spectrum generated for the modulation amplitude used (0.035 cm⁻¹ peak) and for the CO₂ pressure (5.73 mbar for this example) required to match the observed modulated direct transmission level. For each target spectral line the peak-to-peak 2f signal amplitude

(in counts from the analog to digital (A/D) converter) is divided by the observed laser power at line center for that line (also in A/D counts, from the dc spectrum) to obtain the normalized 2f signal level. This process defines the R number for that spectral line, which is essentially a measure of the 2f signal chain gain. Note that an accurate pressure measurement (for a pure gas, or a precisely known abundance of the target gas for an impure sample) and knowledge of the laser modulation amplitude are required for determination of R for each channel. For Mars spectrum analysis a data-processing matrix describing the variation in 2f signal amplitude with total pressure and temperature is consulted to make the necessary corrections for the change in 2f line shape with pressure and temperature (see May [1998] for an example of such a matrix) and to extract the absolute 2f signal amplitude for a given number density of target gas.

Line strengths for the target H₂O lines have been measured by Toth [1994] using high-resolution Fourier transform spectroscopy. Extensive line strength measurements for a strong H₂O line in this same spectral region by May [1998] are in excellent agreement (<2%) with Toth's value and support his absolute line intensities in this region. Net uncertainty in the H_2O line strengths is <4% for the TEGA and MET target lines. At typical Mars ambient pressures (<10 mbar) the pressure-broadened component of the observed line widths for H_2O will be ~10% of the Doppler component. Therefore uncertainties in the CO₂ broadening coefficient for H₂O will not have a significant impact on derived water vapor volume mixing ratios. For CO_2 the line position and intensity data are taken from the 1996 HITRAN database [Rothman et al., 1998] for all isotopes. References there describe how the HITRAN data were assimilated for CO₂ in the 2 μ m region and the expected uncertainties. Line strengths for the CO₂ spectral lines used for both the MET and TEGA spectrometers have estimated uncertainties below 5%. As with H₂O, pressure broadening for CO₂ (self-broadening in this case) is relatively

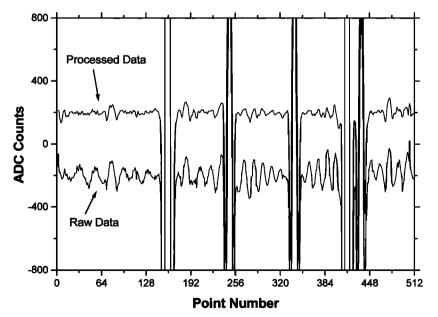


Figure 6. Example of optical fringe reduction for CO_2 via an interative software analysis method. The optical fringes arise from standing waves set up within the laser/detector path and could not be further minimized for the MVACS TDL systems because of insufficient lateral adjustment range for the laser-collimating lens. Signal amplitudes are in A/D counts.

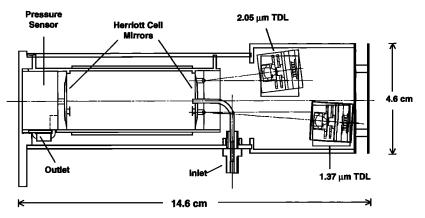
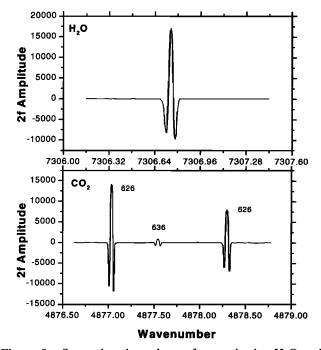


Figure 7. Plan view layout of the TEGA TDLs and Herriott cell. The laser/detector assemblies are located in a chamber that is connected to the insulated (aerogel) Herriott cell but thermally isolated from the Herriott cell itself via a G-10 insulating washer. Gas enters the Herriott cell through a 1/16" OD stainless steel tube and exits at the opposite end of the cell, where a pressure sensor is located. The Herriott cell temperature is stabilized at 308 K to avoid condensation of H₂O.

small at the low pressures expected at Mars. However, it represents a larger fraction of the observed line width for CO_2 owing to the higher molecular weight and the longer wavelength, which combine to reduce the Doppler component of the line width. The Doppler width for CO_2 at 273 K and 4880 cm⁻¹ is 0.0044 cm⁻¹ compared to a self-broadened component of ~0.001 cm⁻¹ at 10 mbar and 273 K.

Minimum detectable number densities for H_2O and CO_2 are listed in Table 1 for both the MET and TEGA TDL spectrometers. These values are based on measurements from single spectra with no spectrum averaging or fringe reduction efforts. Note that the spectral regions are different for the two spectrometers, so the relationships between minimum detectable absorption level (in terms of fractional absorption) and minimum detectable gas number density are different. The base detectable line center absorption level in the TEGA spectra is 8×10^{-4} , while for the MET spectra the minimum detectable absorption level is 4×10^{-4} . These values are an order of magnitude larger than is relatively easily attainable in a properly aligned second harmonic TDL spectrometer and result



1.000 0.995 **TEGA Data** 0.990 Synthetic Transmission 0.985 0.980 0.975 modulated direct 0.970 transmission 0.965 4878.00 4878.10 4878.20 4878.30 4878.40 4878.50 4878.60 3000 2000 1000 Counts 0 **X**-1000 -2000 2f spectral line -3000 4878.00 4878.10 4878.20 4878.30 4878.40 4878.50 4878.60 Wavenumber

Figure 8. Spectral regions chosen for monitoring H_2O and CO_2 for the TEGA TDL spectrometer. The numeric labels next to the CO_2 2f lines identify the CO_2 isotopomers as in Figure 5. A weak 628 line is also present in the spectrum near 4878.0 cm⁻¹, but this line will be observable only for very high levels of CO_2 in the TEGA cell. Signal amplitudes are in A/D counts.

Figure 9. (top) Modulated direct transmission spectrum and (bottom) the corresponding 2f spectrum used to derive the 2f signal chain response number R. Analysis of these spectra defines the quantitative relationship between the observed 2f signal amplitudes and the gas number density for fixed electronic gain factors and laser modulation amplitude.

from the inability to position the collimating lens in the correct position for these systems. Since the fringing levels vary slightly with the measurement conditions (temperature primarily), the values listed are typical of those observed using the flight spectrometers and are based on peak-to-peak fringe levels in the spectra.

The ¹³C¹⁶O₂ and ¹²C¹⁸C¹⁶O isotopomers of CO₂ are present in both MET and TEGA spectral regions, as shown in Figure 5 and Figure 8. On the basis of the minimum detectable absorption levels measured from single spectra, the precision of the ${}^{12}C/{}^{13}C$ and ${}^{16}O/{}^{18}O$ isotopic ratios can be estimated if an assumption is made for the total number density of CO₂. For the MET spectrometer, assuming a 95% CO₂ atmosphere, 7 mbar total pressure, and 240 K temperature, the precision in the isotopic ratios measured from single spectra is $\sim 1-2\%$ for both ${}^{12}C/{}^{13}C$ and ${}^{16}O/{}^{18}O$ since the ${}^{13}CO_2$ and ${}^{12}C^{18}O^{16}O$ spectral lines have approximately equal intensity. Averaging small groups of spectra and applying fringe reduction techniques should improve the precision by at least a factor of 2 and in some cases as much as a factor of 4. Longer-term spectrum averages (over many MET sessions) should lead to significant improvement in the precision of the isotopic ratios since the optical fringes in the spectra average out well over longer time periods. For TEGA the ¹⁶O/¹⁸O ratio will probably not be measureable to better than 30% even for a pure CO₂ sample. The ${}^{12}C/{}^{13}C$ ratio should be measureable to $\sim 10\%$ for a pure CO₂ sample with no spectrum averaging and to \sim 3-4% with extensive spectrum processing. These values can be linearly scaled for lower CO₂ abundances more typical of those expected during an actual TEGA run. Longer-term spectrum averages are not feasible for TEGA owing to the nature of the experiment (i.e., the time dependence of the evolved gases). Again, excessive optical fringe levels in the spectra limit the precision to which isotopic ratios can be determined.

There is a very weak HDO line within the MET spectral region at 7298.1 cm⁻¹ that might be observable for sufficiently high levels of water vapor, optimum spectrum processing, and longer-term spectrum averaging. The calculated line center absorption for this HDO line, using the HDO line parameters of *Toth* [1994], is 4×10^{-5} for a total water vapor number density of 1×10^{14} molecules cm⁻³ at 7 mbar total pressure and 270 K (this number density corresponds to ~500 ppmv) and an assumed D/H ratio that is 6 times greater than on Earth. On the basis of the single-spectrum minimum detectable line center absorption value of 4×10^{-4} , this line would not be observable. However, with multiple spectrum averages over many MET sessions this line may be detectable and would provide a direct measurement of the atmospheric D/H ratio.

The MVACS TDL instruments are the first diode laser spectrometers to be designed, qualified, and flown on a planetary mission. Although significant design compromises were necessary to accommodate these instruments within the MVACS payload, their inherent small size, low power consumption, lack of moving parts, and high detection sensitivity for a wide range of gases make TDL spectrometers viable and valuable tools for future space-borne and planetary instrument payloads. Improvements to the electronics and optical designs, which have already been implemented in prototypes currently being built at JPL for the International Space Station, along with new semiconductor laser sources such as quantum cascade lasers which can operate at wavelengths as long as 17 μ m at room temperatures, should greatly improve instrument performance and utility for space-borne applications of semiconductor laser spectrometers.

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