SPECTRALOGGER: An ultracompact tunable diode laser spectrometer for automated field use

Wolfgang Gurlit, Institute of Environmental Physics, University of Bremen, Germany
gurlit@iup.physik.uni-bremen.de, phone +49421 2187006, Otto Hahn Allee 1, 28359 Bremen

ABSTRACT

A small size tunable diode laser (TDL) spectrometer with dimensions of only 280 x 190 x 130 mm (11 x 7.5 x 5 inch) was built for automated field use. The water-protected package also contains batteries and a data storage device for an independent operation of 15 hours. Mass of the complete instrument is 5 kg. Smallest absorptions recorded in fully automated operation are in the 10^{-5} range. Data is stored as direct absorptions and as derivative as well. The instrument can be equipped with near infrared (NIR) laser diodes depending on target species (e.g. water vapor or methane). A high dynamic range is achieved by periodically tuning the laser over various molecular absorption lines of different line strength using temperature scan. The absorption path is set up using a retroreflector, the pathlength can be between 0.5 meters and 100 meters depending on requirements. The instrument is targeted at reliable and sensitive field measurements in fully automated and unattended mode, including e.g. aircraft and environmental measurements.

1. INTRODUCTION

TDL spectroscopy is a versatile and approved tool for many scientific and - to some extent- environmental and industrial applications. This is especially true when diode lasers in the near-infrared spectral range between 800 and 2000 nm wavelength are used. In this range, overtone and combination bands of many important absorbers like H_2O, CH_4, CO_2, CO, HCL, NH_3, H_2S, HF can be found. Linestrengths are significantly smaller than the fundamental bands in the IR, but this disadvantage can be compensated by a number of advantages that are not available in the more "classic" IR region.

NIR-TDL spectroscopy benefits a lot from the singlemode narrow-bandwidth distributed feedback (DFB) laser designs, whose development was driven by the telecommunication industry. Specialised smaller firms, and sometimes even the labs of the big laser diode suppliers, have developed modified telecom laser diodes that can be offered in many different wavelengths that are of spectroscopic interest. Using new technologies like strained layer architechture, customer specification of the emission wavelength all the way from 0.8 to 2 µm became possible in the mid-90s.

A number of instruments [1-4] has been using these room-temperature laser sources to achieve minimum detectable absorbances (MDA) down to the 10^{-6} range in the lab and typically 10^{-5} range in the field. However, the practical usefulness of these spectrometers often is not limited by their sensitivity but by the complexity of operation. They provide useful and reliable measurements only when operated by skilled scientific personnell and are mostly run by their own developers. Most instruments are "masterpieces" and not designed as a base for a production instrument. For this reason, their application is restricted to special scientific campaigns where these instruments provide valuable but relatively sparse, snapshot-like results.

The general idea of the new instrument described here is to use current NIR-TDL technology in a low-complexity and low cost instrument that can be operated independently on a routine base by standard technical staff. Removing the complexity of most of today´s designs makes adaptation to a great variety of measurement tasks very easy, without compromising too much of the sensitivity potential of the technology. With the widespread use of near-infrared technology operating at room temperature, some bulky and "user-unfriendly" components of the earlier times like cryogenic cooling systems were removed already years ago. However, at least two key-components that require expert attention are still considered necessary and present in most of today´s field-TDL spectrometer designs:

- **multireflection absorption cells** (mostly Herriott-design) require delicate optomechanical adjustments in order to achieve the necessary absorption path length. Most applications [2-4] require absorption path lengths between 10 and 100 meters resulting in more or less the same number of optical reflections on the cell mirrors. The precise adjustment of these mirrors is the key factor number one for in-situ campaign instruments. The high number of reflections results in the need for extreme high reflectivity of the mirrors in order to achieve sufficient optical transmission of typical 1 to 5 %. Contaminations deposited during field use are difficult to remove. Though in some cases Herriott cells proved to be relatively stable over time [2], in general they need a high maintenance level which makes it difficult to operate them on a routine basis during extended periods.

- onboard computer controlling among others, the precise laser emission wavelength. During power-on process, most instruments require operator interaction in order to find the correct emission wavelength (usually found by using a reference cell which contains a defined concentration of the absorber). After manual adjustment of the laser´s operating parameters, a linelock algorithm then can take over control of the laser´s current and temperature to lock the emission wavelength to the absorption line of interest. The standard approach is then to periodically scan the absorption feature by current ramping, while the temperature is kept constant. Simply reproducing the laser diode´s operating (tuning-) parameters temperature and current on power-on does not guarantee the reproduction of the emission wavelength with the accuracy required to record a molecular absorption. The reason for this are, among others, nonlinearities in the lasers response to the tuning parameters.

2. THE LOW-COMPLEXITY APPROACH

The Spectralogger does not contain onboard computer or microprocessor, nor complex optical parts. To put it into operation, only the power switch has to be set to "on" position. In the concept described here, the somewhat difficult situation during power-up of most instruments is overcome by periodically tuning the laser through a temperature interval. The thermal tuning coefficient of DFB lasers in the NIR is typically 0.1 nm or 10 GHz / °C. This means, that with a temperature variation of only 1 °C a complete, pressure broadenend absorption line can be scanned, a task which has always been difficult to achieve with current ramping.

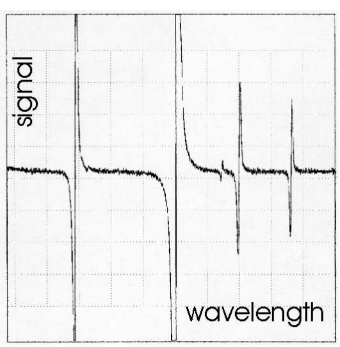

Fig. 1: A scan across five water vapor absorptions with the spectralogger (derivative)

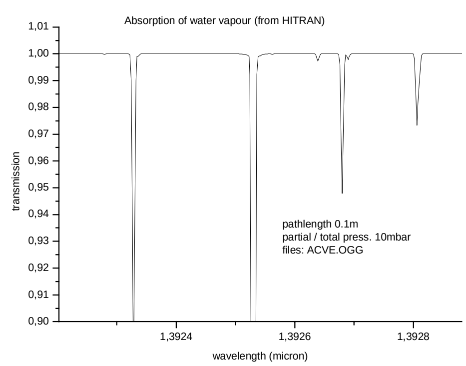

Fig. 2: The same absorptions modelled with HITRAN

The overall temperature tuning range of a typical NIR-DFB laser diode is one to two orders of magnitude larger than the current tuning range. By increasing the scan range to e.g. 5 degrees, a whole group of lines can be scanned. This is achieved with a thermoelectric (peltier) cooling / heating element of 1 watt electrical power and precision analog electronic control circuits. As a result of the large scan range, there is no linelock or other feedback control loop needed. In all tests, the laser safely reached its target wavelength interval using the analog temperature control. Simply by periodically tuning the temperature of the laser diode between e.g. 15 °C and 20 °C, a whole group of water vapour lines can be scanned. This is especially helpful to increase the measurement dynamics. For measurements of relatively high concentrations, a weak absorption can be used to avoid saturation, while for low concentration a stronger line can be used to improve the S/N ratio. A scan across a spectrum of five absorption lines in shown in fig. 1. The data was recorded directly from the Spectralogger´s analog output using an oscilloscope. The same situation modelled with HITRAN can be seen in fig. 2. To achieve a long absorption path without a multireflection cell, the Spectralogger relies on an external retroreflector. This idea was successfully applied earlier by the BLISS-experiment with path lengths of up to 1 km [5].

2.1 Instrument Design

The drawing below (fig. 3) shows the general outline of the TDL spectrometer. It works with a retroreflector instead of a multireflection cell and a data logger instead of an onboard computer. The various system components are described in detail below.

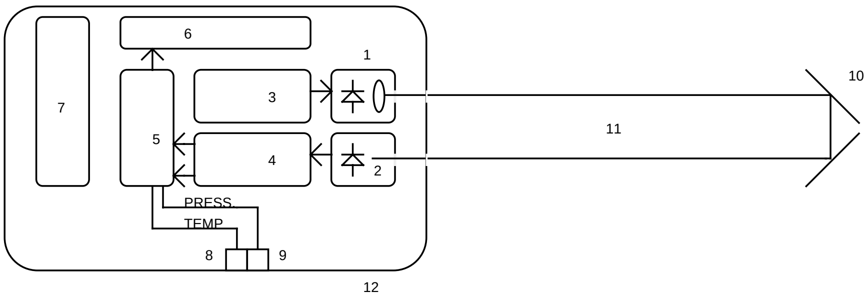

Fig. 3: SPECTRALOGGER design with laserdiode assembly (1), photodiode (2), laser driver and temp control (3), photodiode amplifier and signal conditioner (4), signal multiplexer (5), data logger (6), batteries and power conditioning (7), outside temperature sensor (8), outside pressure sensor (9), cube-corner reflector (10), absorption path (11), water-protected plastic enclosure (12)

The complete instrument is contained in a weatherproof (water protected) industry-standard plastic enclosure of 11 x 7.5 x 5 inches. Inside, all components are installed in a rugged aluminum frame that has an additional function as a heatsink. The mechanical design resists vibration and shock. The only additional component necessary to form a complete spectrometer is the external retroreflector. Lasersource and optical detector are placed close to each other on one side of the box. To form the absorption path, the retroreflector has to be placed in front. The absorption path length is then two times the distance between the instrument and the retroreflector, it can be in the range from 0.5 to 100 meters, which makes it easy to accomodate a great variety of measurement situations. The Spectralogger consists of these modules:

Laser diode assembly (1) with laser diode, collimator, Peltier cooler/heater, laser drive circuits. For the experiments described here, a DFB laser from Sensors Unlimited in TO 5 package was used. Emission wavelength is around 1393 nm, which allows access to a number of water vapor absorptions. Optical power is 3 mW. For beam collimation a commercially available collimator (Melles Griot) installed in an xyz-translator is used. The laser diode sits on top of a small TE-cooler/heater unit, which is equipped with a temperature probe. Excess heat generated by the TE-cooler is transported to the aluminum baseplate. The laser diode is directly mounted on the circuit board of its custom made precision current driver.

Photodiode (2) installed next to the laser assembly. This low-noise Ge PIN photodiode is operated in photovaltaic mode without bias. It receives the optical signal from the laserdiode via the external reflector that forms the optical path. The photodiode is directly mounted on the circuit board of its preamplifier (4)

Laser **temperature and current control unit (3)**. This analog circuit ramps the temperature linear between two set points that can be adjusted each with a precision potentiometer. The temperature range to be scanned can easily be modified to suit many applications. Temperatures accessible lie between 0 °C and 40 °C. The current is neither ramped nor modulated.

Low noise **preamplifier (4)** for the photodiode signal. It delivers the direct absorption signal and a derivative signal which is generated by a realtime differentiation circuit. This signal is of special interest for the retrieval of smaller absorptions (10^{-3} to 10^{-5} range). Both signals are generated in parallel and are recorded by the datalogger (6).

Signal **multiplexer (5)**. As the data logger used in this instrument is a one-channel device, this circuit is needed to multiplex the 6 signals to be recorded. They are a) absorption direct mode, b) absorption derivative mode, c) laser temperature, d) outside temperature, e) pressure, f) dark (background, laser off) signal. In fact, it uses 16 channels to provide higher sampling rates for the absorption signals (8 channels derivative mode, 4 channels direct absorption mode) than for the environmental and houskeeping signals (one channel each).

Data logger (6). This is a small-sized commercial device with 16 bit A/D conversion, watertight packaging in a steel tube and independent power. It is designed for operation under harsh environmental conditions. Operation is synchronized to the multiplexer. Programming and data download works via an IR-link. The device holds 1 million data points of 16 bits each. With the data rate of 20 per second normally used, recording is possible during approximately 14 hours until the memory is full.

Batteries & power conditioning (7). The Spectralogger operates from 8 standard "D" cells of 1.5 volts, 18 Ah each, available almost everywhere in the world. The total capacity of 216 Wh of this battery pack allows at least 15 hours of continous operation. These alkaline batteries were tested in our lab to work at ambient temperatures between –20 °C and +50 °C and in a pressure range from 1 mbar to 1000 mbar. Battery life can be extended by 50% in applications where the electric heater for the retroreflector is not needed. Via a watertight connector, an external power supply can be connected. The Spectrologger draws current from the external supply if the voltage is higher than the internal battery voltage. The battery or external voltage is adapted, filtered and stabilised by DC-DC converters and stabilising circuits to enable reliable operation.

Outside **temperature and pressure sensors (8, 9)** and associated signal conditioning. P and T are measured by calibrated sensors in the range from –50 °C to +150 °C (T) and 0 to 1000 mbar (P).

Corner cube **reflector (10)**. This device works as a retroreflector that always reflects the outgoing beam parallel to the incoming beam. The use of this reflector greatly relaxes the requirements for the optical adjustments when the instrument is set up. As long as the collimated laser beam hits the reflector (diameter is 2.5 inch), the beam will be reflected back onto the photodiode. For very long absorption path lengths the use of an even greater reflector could be advantageous. As the collimated laser beam is reflected on only two optical surfaces of the reflector, optical efficiency of the absorption path can be much greater than with a multireflection design. As a result, light levels received by the photodiode (2) are relatively high, making the instrument quite insensitive to stray light. Further, the S/N ratio of the received optical signal is improved. The reflector is equipped with an electrical heater. If needed for specific applications, by heating the unit above ambient temperature, the condensation of water, which would interrupt the optical path, can be avoided.

Industry standard **plastic box (12)** with sealed cover, that contains all the components with the exception of the retroreflector.

3. PRACTICAL OPERATION

The unit must be equipped with a NIR laser diode that covers the wavelength region for the absorbing species to be measured. For our experiments, we used laser diodes from Sensors Unlimited emitting around 1393 nm (for water vapor) and 1653 nm (for methane). Upper and lower temperature limit for the temperature scan have to be adjusted only once in the lab. First thing in the field then is to set up the absorption path. This is simply done by firmly installing the spectralogger main unit and the retroreflector at a distance that is long enough to produce absorptions in the 10^{-2} to 10^{-5} range but short enough to prevent saturation of the absorption lines. The pathlength must be precisely known in order to apply Beer´s law for the calculation of gas concentrations. After installation, the xyz-translator of the laser diode´s collimator may need to be readjusted to bring the best level of reflected light onto the photodiode. The start time of the data logger can be programmed with a notebook-PC using infrared communication. Data transfer from the logger after data acquistion also works via infrared interface. The data can then be converted from binary format to ASCII and plotted or processed by standard software.

4. RESULTS

Some spectra of water vapor around 1393 nm recorded with the Spectralogger in a vacuum chamber are shown below in fig. 5 and 6. Both plots show raw data directly delivered by the Spectralogger with no co-adding, smoothing, background subtraction or other processing step applied. While fig. 05 shows the direct absorption mode, the same situation but in derivative mode is shown in fig. 06. The line on the left side of each of the two figures (1392.81 nm) corresponds to an absorption of 3 x 10^{-3} (I_0 was 510 mV). As a result of the flat baseline typical for derivative signals, the stronger absorption at 1392.53 nm, though clipped, could also be displayed in the same plot, which was not possible in the direct mode.

Acquisition time for the spectrum in fig. 05/06 was 40 seconds. This time is defined by the relatively slow temperature scan.

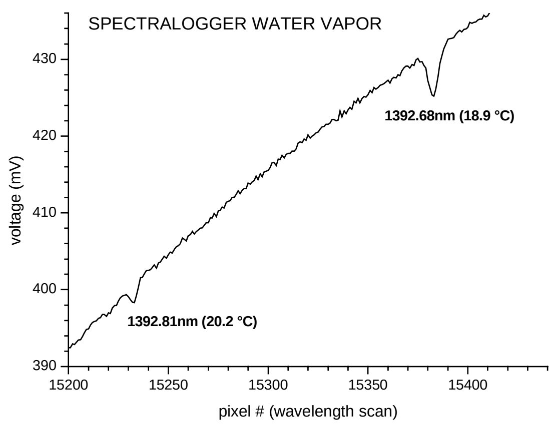

Fig. 5: A scan across two water vapor absorptions in direct mode

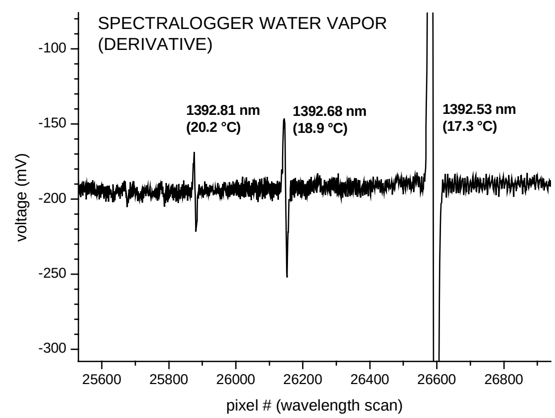

Fig. 6: Water vapor absorptions in derivative mode

5. CONCLUSION, FUTURE DEVELOPMENT

A general limitation of the concept of periodic temperature tuning of the laser diode is the tuning speed, which is low in comparison to current tuning applied in most other instruments. While with some technical improvements the acquisition time for a complete spectrum can be reduced from 40 seconds (now) to 10 seconds, with current ramping a single line can easily be scanned in one millisecond. However, scanning of a group of lines like shown here with the Spectralogger, is very difficult and in most cases even impossible with current tuning. The current tuning coefficient of DFB lasers is too small, and the tuning range is limited between the laser´s threshold and the overload limit causing device damage.

In many industrial and environmental applications, the temporal resolution of 10 to 40 seconds should be perfectly sufficient. For other applications such as gas combustion monitoring, the temporal resolution will not be good enough. A faster thermal scan however would be possible using pulse-heating of the diode laser with another focused laser source. Using this technique, rapid temperature tuning (RT) has been demonstrated on a millisecond scale [6]. Practical aspects of this technique like possible degradation of the laser diode by the cyclic rapid heating and cooling however remain to be investigated.

The "classic" thermal scan used on our instrument showed another problem that needs to be solved. The laser diode is installed inside a small copper block that sits on top of a thermoelectric cooler. Thermal expansion of (mainly) the TE cooler results in a small periodic misalignment of the laser beam, as the laser diode is performing a micro-movement, but the collimater stays in place. As a consequence, a large thermal scan like shown in fig. 06 cannot be made if the distance between the instrument and the reflector is more than 10 meters, because the laser beam may occasionally miss the reflector. This problem can be solved with an improved design of the laser diode assembly. The design used so far, and one better arrangement are shown in fig. 7.

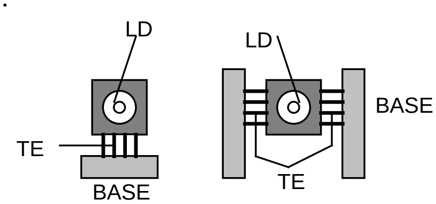

Fig. 7: Thermal expansion of the TE cooler causes micromovement of the laserdiode (LD) and subsequent beam movement during the temperature scan (left). A simple improvement avoiding tilting and misalignment is shown on the right side.

A second version of the spectralogger is currently being assembled. In addition to the improved arrangement of the TE cooler / diode unit proposed in fig. 07, it uses a dual path background absorption scheme and a more modular design of the optomechanics and the electronics. Also, an autocalibration feature already sucessfully used by us in another instrument (a ballonborne TDL spectrometer used on a stratospheric ballon in the SCIAMACHY satellite instrument validation, to be reported elsewhere) will be implemented in the spectralogger to further ease operation and data processing.

The general concept of thermal scan and the absorption path using a retroreflector will stay unchanged. The new unit will consume less power and operate longer from the same set of household batteries. The spectralogger does not intend to replace the usual designs of today´s field instruments. However it clearly intends to bring the advantages of TDL-spectrocopy into new fields of routine application where the expert scientist operating today´s instrument is not present.

6. REFERENCES

1) D. M. Sonnenfroh, W. J. Kessler, J. C. Magill, B. L. Upschulte, M.G. Allen, J. D. W. Barrik, "In –situ sensing of tropospheric water vapor using an airborne near-IR diode laser hygrometer", Applied Physics B 67, 275-282 (1998)

2) Randy D. May, "Open-path, near-infrared tunable diode laser spectrometer for atmospheric measurements of H_2O", J. of Geophys. Res., Vol.103, No. D15, 19161-19172 (1998)

3) G. Durry, G. Megie, "Atmospheric CH_4 and H_2O monitoring with near-infrared InGaAs laser diodes by the SDLA, a balloonborne spectrometer for tropospheric and stratospheric in situ measurements", Applied Optics, Vol. 38, No. 36, 7342-7354 (1999)

4) S. I. Chou, D. S. Baer, R. K. Hanson, "Diode laser absorption measurements of CH_3Cl and CH_4 near 1.65 μm", Applied Optics, Vol. 36, No. 15, 3288-3293 (1997)

5) C. R. Webster, R. D. May, "Simultaneous in situ measurements and diurnal variations of NO , NO_2 , O_3 , jNO_2 , CH_4 , H_2O , and CO_2 in the 40- to 26-km Region using an open path tunable diode laser spectrometer", J. of Geophys. Res., Vol.92, No D10, 11931-11950 (1987)

6) S. T Sanders, D. W. Mattison, J.B. Jeffries, and R. K Hanson, "Rapid temperature tuning of a 1.4-μm diode laser with application to high-pressure H2O absorption spectroscopy", Opt. Letters, Vol.26, No.20, 1568-1570 (2001)