European Geosciences Union
General Assembly 2011
Vienna | Austria | 03 – 08 April 2011

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EGU 2011 SC2/IG16 Short Course

on

Laser-based Isotope Ratio Analyzers: The User Perspective

Thursday April 7, 14:30 – 18:00, room 25

Conveners:

Peter Werle and Erik Kerstel

Karlsruhe Institute of Technology

Université Joseph Fourier

Laboratoire interdisciplinaire de Physique

Laser-based Isotope Ratio Analyzers: The 3rd EGU Short Course

2009: Short Course by Erik Kerstel and Livio Gianfrani who discussed the fundamentals of the relevant optical techniques, in a manner accessible to the non-specialist, as well as sample handling and calibration issues that are specific to the laser instrumentation.

2010: Short Course on Laser-based Isotope Ratio Analyzers with contributions from the leading commercial suppliers.

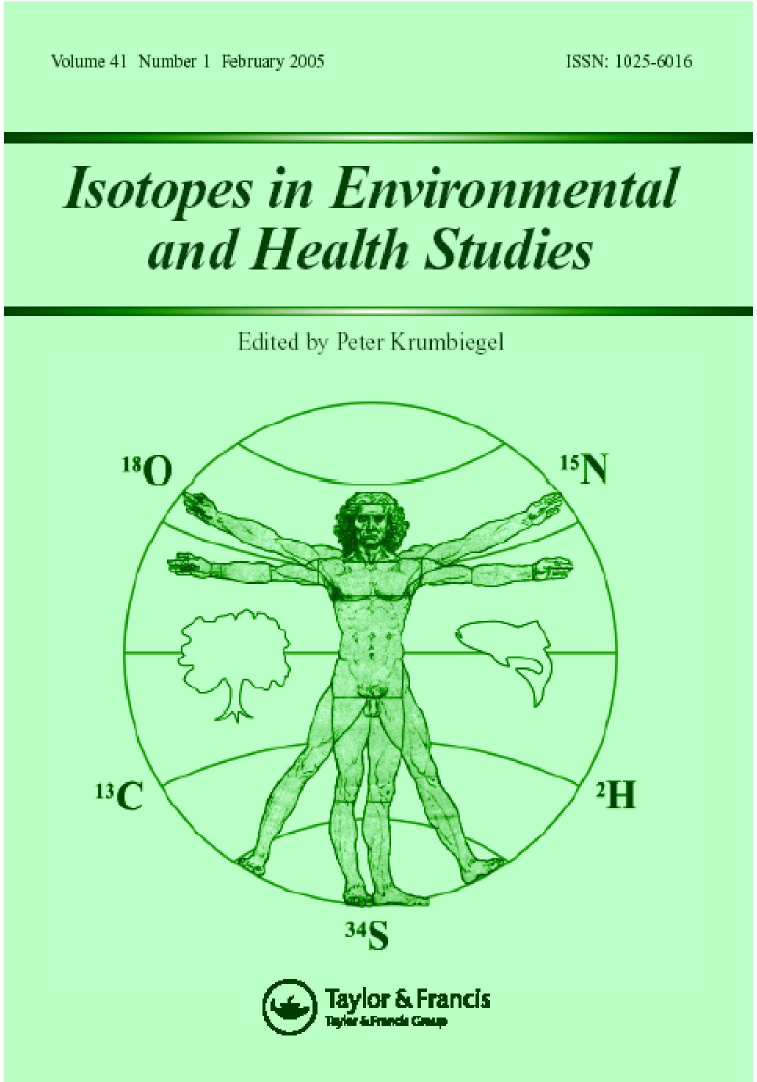
2011: In this Short Course we will take a critical look at recent developments from the end-user perspective. What is needed to successfully operate these instruments in order to obtain reliable data? Where are the pitfalls? The Short Course is organized around relatively short, but focused presentations by experienced users of laser analyzers from **Aerodyne Research, Campbell Scientific, Los Gatos,** and **Picarro**.

Laser-based Isotope Ratio Analyzers: The Issues

- Isotope scale calibration, two point scale fixation and contraction/expansion
- Amount/concentration dependence
- Memory effects
- Matrix effects
- Water vapor measurements: calibration against liquid standard materials
- Intercomparison between instruments and laboratories (ring tests)!
- Trained operator? In isotope issues certainly, but what about the ‘black’ box?
- Supply of standard materials in a form adapted to laser instruments
- Sensitivity of the instruments – how much material is needed (nanomols?)
- Field applications, environmental impacts, temperature gradients and speed of temperature changes, …
- Good laboratory practices, reporting uncertainties

Laser-based Isotope Ratio Analyzers: Programme

14h30-14h40	Erik Kerstel (UJF Grenoble) or Peter	Introduction
14h40-15h00	Eric Pili (CEA Paris)	Assessment of the LGR CO_2 isotope analyzer to investigate gas transfer in geological media
15h00-15h20	Nickolas Brüggemann (FZ Jülich)	Combined application of the Campbell TGA200 CO_2 and the Picarro H_2O isotope analyzers
15h20-15h40	Patrick Sturm (ETH Zurich)	Using Aerodyne and Los Gatos analyzers to measure biosphere-atmosphere fluxes of CO_2 and H_2O isotopes (Aerodyne / Los Gatos)
15h40-16h00	Manfred Groening (IAEA Vienna)	Calibration issues for d2H and d18O data produced by laser systems
16h00-16h45	COFFEE BREAK	DISCUSSIONS
16h45-17h05	Lisa Wingate (U of Cambridge)	Measuring the seasonal d13C and d18O signals of ecosystem CO_2 fluxes using a fast response tunable diode laser spectrometer. (Campbell)
17h05-17h25	Daniela Polag (MPI Mainz)	Measurements of stable carbon isotopes of methane and CO_2 in anaerobic digesters using laser absorption spectroscopy (Los Gatos)
17h25-17h45	Bela Tuzson (EMPA, Duebendorf)	The road towards high-precision isotope ratio measurements by QCLAS
17h45-18h05	Brent Newman (IAEA, Vienna)	Laser-based isotope ratio analyzers, tips and tricks from the IAEA Hydrology Section
18h05-18h20	Peter Werle (KIT, Karlsruhe)	Summary, messages, and concluding remarks.



The Editors,

Gerhard Strauch & Peter Krumbiegel,

invite you

to publish your contribution at the EGU 2011

in

Isotopes in Environmental and Health Studies

The journal deals with all aspects of non-radioactive isotope application in environmental and health studies

- **Investigations using variations in natural isotope abundance** (isotope ecology, isotope hydrology, isotope geology).
- **Stable isotope tracer techniques** to follow the fate of certain substances in soil, water, plants, animals and inthe human body.
- **Diagnostic (stable) isotope application** in medicine.
- **Isotope effects, tracer theory, and mathematical modeling** of isotope based environmental cycles.
- **Isotope measurement methods and equipment** with respect to environmental and health research.
- **Ionogenic radiation exposure** and its effects on all living matter as well as radiation protection and natural radiation.

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Submitting manuscript: http://mc.manuscriptcentral.com/gieh

FLAIR 2011 – International Conference – September 13–17, 2011 – Murnau, Germany

http://imk-ifu.fzk.de/flair/

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International Conference

FLAIR 2011 - Field Laser Applications in Industry and Research

September 13-17, 2011 - Conference Center, Murnau, Germany

Guests & Speakers of this SC may still submit contributions to

Stable Isotope Ratio Infrared Spectrometry

Display a menu

Field laser applications in industry and research

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Lasers and Optics

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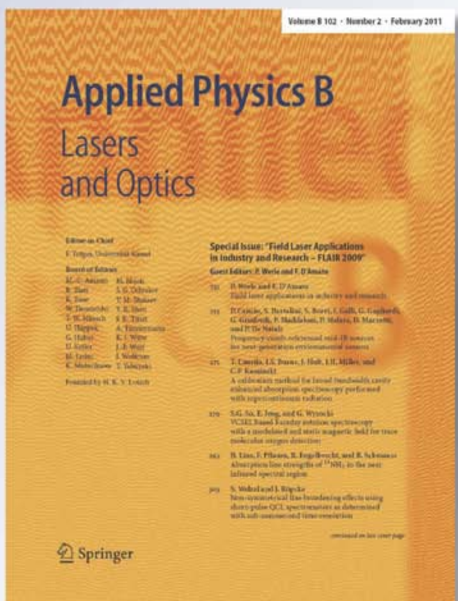

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Applied Physics B
Lasers and Optics

Accuracy and precision of laser spectrometers for trace gas sensing in the presence of optical fringes and atmospheric turbulence

P. Werle

Received: 22 March 2010 / Revised version: 2 July 2010

Abstract Spectroscopic techniques are increasingly used for field laser applications in industry and research. Under field conditions complex gas sensors cannot be considered as stable and therefore drift characterization is a key issue to distinguish between sample data and sensor drift. In this paper the history of von Neumann's two-sample variance and Allan variance stability investigations in the field of frequency metrology and the relationship to wavelet analysis are reviewed. The concept has been used to characterize accuracy and precision of spectroscopic data in the time domain and practical guidelines for the interpretation of σ/τ plots are presented. Two topics relevant for spectroscopic measurements are discussed: First, the optical fringe effect, which is present in any spectrometer, limits the precision and accuracy of spectroscopic measurements by forming time dependent background structures superimposed to the signal under investigation. The two-sample variance is used to characterize optical etalons and long-term drift using σ/τ plots. Second, the short-term instrument stability characteristic in the presence of atmospheric turbulence is discussed. This is important for laser-based gas monitors measuring the turbulent transport of trace gases between the biosphere and the atmosphere using the eddy-covariance technique. It will be shown how the spectral characteristics of turbulence in the Kolmogorov inertial subrange can be identified in the time domain and how the effect of optical fringes can be separated from atmospheric signals.

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1 Introduction

Modern spectroscopic techniques based on semiconductor lasers are increasingly used for field laser applications in industry and research [1–8]. Under field conditions these complex measurement devices cannot be considered as stable and drift characterization is still a key issue to distinguish between sample data and sensor drift. The question is how drift in such instruments can influence precision and accuracy of the measurement. In 1816 Gauss [9] described the distribution of observation to be normal with a probability density function (PDF) proportional to $h \cdot \exp(-h^2x^2)$. He named the positive constant h the precision, which later was replaced by the standard deviation $\sigma = 1/\sqrt{2}h$. In general, precision and accuracy describe the relationship between a measured value and the true value. To investigate precision and accuracy a series of successive measurements of a known concentration have to be recorded. When these data are then plotted as a frequency distribution it is expected from the central limit theorem, that the acquired data are normally distributed [10]. The mean occurs at the center of the distribution, and represents the best estimate based on all of the measured data. The standard deviation describes the width of the distribution as the variation that occurs between successive measurements. The amount of shift from the true value is called the accuracy of the measurement. The width of the distribution indicates that individual measurements may not agree well with each other. This precision of the measurement is expressed by quoting the standard deviation. In cases where a measurement that has a high accuracy, but a low precision, the histogram is centered over the true value, but the distribution is very broad. Although the measurements are correct as a group, each individual reading is a poor measure of the true value. Poor precision results from random noise or errors, which change each time the measurement is repeated and averaging several measurements