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Trace gas and δ^{13}C - CO_2 analysis by FTIR spectroscopy

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Fourier Transform Infrared (FTIR) spectroscopy is a versatile tool for gas analysis. Applications are widespread from real-time measurement of industrial processes to environmental monitoring of trace gases [1, 2]. The quality of the analytical result, however, is strongly dependent on task-specific optimization of the system which includes hardware configuration, quantification algorithm and calibration strategies.

We developed a method based on a portable, commercially available, 0.5 cm^{-1} resolution FTIR spectrometer which allows simultaneous on-line analysis of multiple trace gases (CO_2, CH_4, N_2O, CO) as well as the $^{13}C/^{12}C$ isotopic ratio of atmospheric CO_2 (δ^{13}C - CO_2). The analytical setup was improved to reach high temperature and pressure stability and an exceedingly good spectral signal to noise ratio. Our method requires no sample preparation other than optional drying and can be applied directly to ambient air. For δ^{13}C - CO_2 we designed a calibration procedure that is distinctly different from the concepts published so far [3, 4], using a set of multicomponent standards that were prepared from CO_2 emission sources with characteristic isotopic composition and quantified by Isotope Ratio Mass Spectrometry (IRMS). For quantification a robust partial least square (PLS) algorithm was used. For the trace gases validation was performed during an inter comparison study at a measuring site of the Swiss National Air Pollution Measuring Network (NABEL) achieving a precision between 0.1 - 0.3 % for CO_2, CH_4 and N_2O, and 0.9 % for CO. Laboratory results for δ^{13}C - CO_2 are very promising with a precision (Allan variance) of 0.3 $\%_{\circ}$ showing its potential to study environmental processes with distinctive isotopic signatures.

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