Geophysical Research Abstracts
Vol. 20, EGU2018-14875-3, 2018
EGU General Assembly 2018


# PTR-MS inter-calibration study at Cabauw

Rupert Holzinger (1), Ralf Tillmann (2), Martin Breitenlechner (3), Baptiste Languille (4), Sebastien Dusanter (5), Jordan Krechmer (6), Leigh Crilley (7), Eiko Nemitz (8), David Worton (9), Arnoud Apituley (10), Felipe Lopez-Hilfiker (11), Simon Schallhart (12), Joe Acton (13), Kangming Xu (1), Lauriane Quéléver (12), Alexander Zaytsev (3), Sergej Wedel (2), and the PICAB team

(1) Utrecht University, Institute for Marine and Atmospheric research Utrecht (IMAU), Physics and Astronomy, Utrecht, Netherlands (r.holzinger@uu.nl), (2) Forschungszentrum Jülich, Germany, (3) Harvard University, USA, (4) LSCE, Chimie Atmospherique Experimentale, France, (5) Atmospheric Sciences and Environmental Engineering (SAGE), IMT Lille Douai, France, (6) Aerodyne Inc, USA, (7) University of Birmingham, UK, (8) Centre for Ecology & Hydrology , UK, (9) National Physical Laboratory, UK, (10) Royal Netherlands Meteorological Institute, (11) Tofwerk AG, Switzerland, (12) University of Helsinki, Finnland, (13) University of Lancaster, UK

In September 2017 we conducted the Proton-transfer-reaction mass-spectrometer (PTR-MS) Intercomparison campaign in CABauw (PICAB) as part of the European infrastructure program Actris-2. Eleven PTR-MS instruments operated by European and US groups measured for two weeks the ambient air composition at the CESAR observatory near Cabauw, Netherlands. All instruments were subjected to a new calibration procedure that comprised a sequence of 50 injections of calibration gas through a sample loop in less than 10 minutes. The calibration gas was custom manufactured by the National Physical Laboratory (NPL), UK, and contained compounds in the m/z range 33-371 Da.

The participating PTR-MS instruments covered a broad range of different makes and types with sensitivities covering the range 2-5E4 cps/ppb. Despite the huge difference in performance (over four orders of magnitude), the mixing ratios calculated based on kinetics in the drift tube deviated typically less than +/-30% of the calibrated concentrations. This results confirms that PTR-MS reliably quantifies concentrations of organic compounds for which calibrations are not feasible (e.g. unknown oxidation products). However, in this respect a proper characterization of the mass dependent transmission efficiency is critical.

The calibration sequence included calibration gas injections in dry and in humidified zero air, which allowed constraining the influence of humidity on the sensitivity for individual compounds. Since the humidity changes the balance between hydronium and hydronium-water clusters the sensitivity is expected to change for compounds that react less efficient with hydronium-water clusters. Our results showed qualitative agreement with published values for the humidity dependence. However, for some instruments the values were outside the range that was expected based on this idea, because of inhomogeneities in the E/N parameter, most likely in the transfer region between drift tube and mass spectrometer.

We conclude that the new calibration procedure (i) directly provides sensitivities of the compounds in the calibration gas, (ii) allows calculating concentrations of uncalibrated compounds by constraining the mass dependent transmission efficiency, (iii) enables for several quality assurance methods, and (iv) holds the potential of fully automated, fast calibrations, which will be an important asset for future field deployments.