5.021 Evaluation of Selected Ion Flow Tube Mass Spectrometry for VOC concentration and emission determination in Beijing - Automation and Calibration considerations..

Presenting Author:
Marvin Shaw, Wolfson Atmospheric Chemistry Laboratories, University of York, marvin.shaw@york.ac.uk

Co-Authors:
jim Hopkins, Wolfson Atmospheric Chemistry Laboratories, University of York
Adam Vaughan, Wolfson Atmospheric Chemistry Laboratories, University of York
Rachel Holmes, Wolfson Atmospheric Chemistry Laboratories, University of York
Freya Squires, Wolfson Atmospheric Chemistry Laboratories, University of York
Lucy Carpenter, Wolfson Atmospheric Chemistry Laboratories, University of York
Ally Lewis, Wolfson Atmospheric Chemistry Laboratories, University of York
Joe Acton, Lancaster Environment Centre, University of Lancaster
Nick Hewitt, Lancaster Environment Centre, University of Lancaster

Abstract:

Volatile organic compounds (VOCs) are emitted from a variety of anthropogenic and natural sources to the earth's atmosphere with their concentrations in air being affected by numerous chemical and physical processes. An ability to selectively quantify VOC concentrations and emissions in both urban and rural environments is of importance to understand and characterise the sources and sinks for induvial VOCs.

To provide a real-time analytical method for the detection of a wide range of VOCs, Spanel and Smith pioneered the analytical application of a portable selected ion flow tube mass spectrometry (SIFT-MS) in 1996. SIFT-MS utilizes known ion-molecule reactions of mass-selected reagent ions with an analyte. The mass-selected reagent ions (H3O+, NO+, and O2+) are introduced into a flow tube at low energy into a carrier gas where they undergo chemical reactions with analytes in the gas sample that is drawn directly into the SIFT-MS flow tube. The availability of NO+, and O2+ enables the measurement of compounds that do not react with H3O+ (e.g., light hydrocarbons, halogenated and inorganic species) and also facilitates the identification of compounds that cannot be differentiated on the basis of H3O+ reactions alone. The switching time of the reagent ion mass filter is sufficiently fast that essentially simultaneous measurements with all three of these reagent ions can be carried out. The ensuing reagent ion-analyte ion-molecule reaction enables identification of the analyte in seconds and provides quantitation from the ratio of counts of the analyte product ion(s) relative to the reagent ion.

In this research we describe the development, optimisation and evaluation of an experimental autonomous air quality monitoring system based upon the Voice 200 Ultra Selected Ion Flow Tube mass Spectrometer (SIFT-MS), and subsequent VOC compound mixing ratio and eddy co variance flux determination during its deployment in Beijing.