Development of a Mobile Mass Spectrometry Laboratory and Data Management Package for Comprehensive Online Chemical Analysis and Real-time Geospatial Mapping

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The release of volatile organic compounds (VOCs) into the environment from anthropogenic sources can have an adverse impact on human and environmental health, degrading air quality locally and regionally. Because the distribution of VOCs can vary widely over time and space, discrete sampling strategies often fail to capture variability, which can be important when it comes to predicting human exposure, dealing with emergency response and informing adaptive sampling strategies.

Described are hardware and software developments associated with a mobile mass spectrometry (MS) laboratory. The laboratory incorporates two complimentary MS systems ruggedized for mobile deployments and continuous operation in a moving vehicle. A cylindrical ion trap capable of tandem MS, has been modified with a membrane inlet and employed for nonpolar volatile organic compounds at low ppb levels. A proton transfer reaction time-of-flight MS is employed for the detection of polar VOCs at parts per trillion levels. The mobile lab also includes several optically based sensors for specific gases including NOx, O_3, CO_2, CH_4 and H_2O.

Sensor data will be handled by BCA Underway (Beaver Creek Analytical, Lafayette, CO) which enables data logging and visualization for 10 arbitrary serial devices. Wind direction is derived from GPS and anemometer vector data for plume tracking. Additionally, MS data files are duplicated to a server in a file format that allows a primary user computer to access data from all instruments and produce timeseries, satellite maps or KML map files in real time.

Preliminary results from field campaigns in and around rural, urban and industrialized areas on Vancouver Island and in Metro Vancouver (BC, Canada) are presented. Geospatial maps of chemical concentration of trace gases generated in real time using BCA Underway are discussed.

Recent progress to identify sources using full scan mass spectra in a non-targeted chemometric approach will also be presented.