Real-time Quantification and Geo-spatial Mapping of Volatile Organic Compounds (VOC) and SemiVolatile Organic Compounds (SVOC) by Tandem Mass Spectrometry

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A miniature cylindrical ion trap mass spectrometer was modified to include a membrane inlet with atmospheric and aqueous sampling capabilities. The membrane inlet allowed for continuous online sampling on mobile platforms. To aid quantification of multiple VOC and SVOC analytes, several modification were developed: 1) the inclusion of an internal standard delivery system, 2) the addition of mu-metal to shield the instrument from varying magnetic field vectors, and 3) the addition of multiple interlaced MSMS/Fullscan spectra. Continuous data collection enables the capture of transient events that may be missed or under represented by grab sampling strategies, provide improved data density for on-site assessments and real-time information to support decision making. Significant efforts were directed at developing the technical infrastructure necessary to enable adaptive sampling in a user-friendly manner. For example, Labview was used to integrate GPS data, mass spectrometer spectra, meteorological data, and meta-data. To take advantage a hierarchal and network-friendly data structure, Google Earth was used to present color-based map trackpoints. Sample data sets presented were collected in western Canada in 2010-2012 and compared to discrete whole-air samples analyzed by state of the art laboratory techniques.

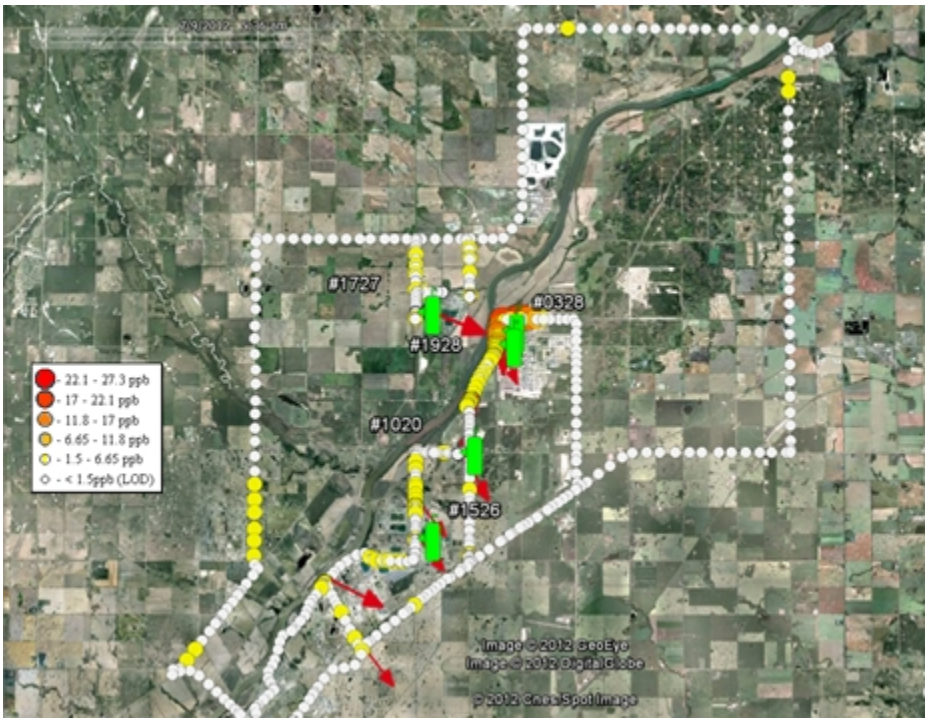

Figure 1. Benzene MS data collected in Fort Saskatchewan, AB. Fugitive emissions from heavy industry resulted in detections significantly above the detection limit (~1 ppb).