Detection of Explosives at a Formerly Used Defense Site with a Portable SPME/GC-Cylindrical Ion Trap Mass Spectrometer

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Long term monitoring of the environment is required to demonstrate successful remediation and regulatory compliance at hundreds of Department of Defense sites. Sampling, shipping, and analysis represent nearly 75% of the total costs associated with long term monitoring, which may be required for 30 or more years. Transportation costs can be reduced or avoided entirely and analytical costs can be minimized with use of field analytical methods, but many current field methods produce screening data that are not acceptable for regulatory purposes. The goal of this work is to develop and demonstrate a field analytical method for determination of explosives that will provide definitive data for regulatory decision making.

An analytical method for detection of semi-volatile analytes including explosives was developed first in the laboratory with a Griffin Analytical Technologies Minotaur 300 cylindrical ion trap (CIT) mass spectrometer prior to field work at a formerly used Department of Defense site. The CIT was interfaced to a solid phase micro-extraction (SPME) inlet and Restek RTX-TNT heated gas chromatography column. SPME fibers were used for analyte pre-concentration and enabled extraction from water without use of solvents and with only 30 mL sample volumes. Chromatographic retention times and characteristic mass spectra permitted confident identification of target analytes and separation from interferences. Operation in the MS/MS mode provided additional confirmatory information on the analytes of interest. Optimal concentration on the SPME fiber depended on fiber type, extraction time, stir speed, temperature, vortex offset position, and salt concentration. Optimal detection parameters also depended on column length and the temperature ramp program. The different targets analytes included in the traditional EPA method for fixed laboratory analysis of explosives, SW-846 Method 8330, showed varying response to SPME concentration and detection on the CIT system.

Analyses were performed in the field at the formerly used Department of Defense site by using a Griffin Analytical Technologies Minotaur 400 CIT mass spectrometer. Water samples were collected from monitoring wells, extracted with SPME fibers, and then analyzed immediately. Results for each sample were obtained in triplicate. To evaluate the accuracy and comparability of the field method, 500 mL samples were transported overnight to our fixed laboratory for analysis by SW-846 Method 8330. Results of the field analysis and corresponding laboratory results will be presented.