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Occupational and Environmental Exposures of Skin to Chemicals - 2005

Abstract for Poster 8

Analytical chemistry of metalworking fluids for dermal and inhalation toxicology studies

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In support of a National Toxicology Program (NTP) study on metalworking fluids (MWF), NIOSH was provided samples of the fluids being tested in that study [NTP 2004]. Aliquots of these fluids were shared with NIOSH researchers for local lymph node assays (LLNA), skin penetration tests, and chemical analyses. Currently, there is no NIOSH method or literature method for the separation and identification of the major components in a MWF mixture. A method for their analysis is described and preliminary results are reported. The analytical results of this method will provide data to researchers of the NTP, LLNA, and dermal penetration studies and likely impact their conclusions.

Liquid and gas phase chromatographic methods were used to characterize the composition of these complex mixtures. The major components in MWFs were separated by high performance liquid chromatography (HPLC) and detected by both ultraviolet (UV) absorption and evaporative light scattering detection (ELSD). The UV detector is a non-destructive specific detector that does not detect all the components, while the ELSD is a destructive "universal detector" capable of detecting most compounds. The ELSD response is a function of analyte mass, and therefore peak areas in a chromatogram reflect the relative abundance of a component in the MWF. The ELSD was used to locate the major components in a MWF with respect to UV-ELSD active internal standards.

A semi-preparative HPLC-UV system was then used to concentrate and fractionate the major components of the MWFs using the UV-ELSD active internal standards as retention time benchmarks to locate collection windows for the major components. The effluent was collected into fractions, and then analyzed by gas chromatography with mass spectrometry (GC/MS). The mass spectrum of each component was matched against the National Institute of Standards and Technology (NIST) spectral library for identification, and, if desired, confirmed experimentally with standards. The HPLC fractions were subjected to further analytical techniques like GC-atomic emission detection, if further confirmation was needed.

The table below contains analytical results from one of the MWFs being studied. The material safety data sheet (MSDS) identified two chemicals in the MWF. The GC/MS analyses of the 11 fractions identified 17 chemicals.

Table. GC-MS identified MWF components in one MWF sample.

Fraction #	Identification	Identified in MSDS
1	✓ Triethanolamine	YES
	Triethanolamine borate	NO
	Hexamethylamine	NO
2	Propylene glycol ethers	NO
3	98-55-5 (+)-.alpha.-Terpineol (p-menth-1-en-8-ol)	NO
4	✓ 4-Chloro-3-methylphenol	NO
5	2-(4-(1,1,3,3-tetramethylbutyl)phenoxy) ethanol	NO
6	26764-25-0 9,12-Octadecadienoic acid	NO
	✓ Hexadecanoic acid	NO
	Tetradecanoic acid	NO
	Chloroparaffin	NO
7	Methyl ester 9,12-octadecadienoic acid	NO
8	Methyl ester 9-octadecanoic acid	NO
9	Methyl ester hexadecanoic acid	NO
	Methyl ester 9-octadecenoic acid	NO
	Methyl ester octadecanoic acid	NO
11	Mineral Oil	YES

The analytical method provided chemical composition information on commercial metalworking fluids not available in the manufacturers MSDS. Individual chemical components of MWF can now be identified by molecular formula, molecular structure, and CAS number. This kind of information will allow for the study of the toxicology properties of individual chemical components within MWFs.

References

NTP [2004]. National Toxicology Program; call for public comments on 21 substances, mixtures and exposure circumstances proposed for listing in the report on carcinogens, twelfth edition. Federal Register 69(97): 28940

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This conference follows the success of the first [International Conference on Occupational and Environmental Exposures of Skin to Chemicals: Science and Policy](#), which was held near Washinton, DC, in September, 2002.

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