



Project Summary

Field Demonstration for Mobile FT-IR for Detection of Volatile Organic Chemicals

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A mobile laboratory is now available to measure toxic compounds in the atmosphere. The mobility of this unit allows access to many sites in the continental United States. When this laboratory arrives at a designated site, a high resolution Fourier transform infrared (FT-IR) instrument is used to measure the toxic materials, or volatile organic compounds, in the atmosphere. The site could be a landfill, lagoon, industrial site, chemical spill or any area where atmospheric pollution occurs. The FT-IR instrument is capable of identifying and quantifying atmospheric molecules at the parts per billion (ppb) level. The path observed by this instrument could be as small as a few meters, or as large as 600 meters in length, nearly 2,000 feet. Recently, the chemicals emitted at an industrial site have been identified at distances of up to 0.3 mile.

This Project Summary was developed by EPA's Environmental Monitoring Systems Laboratory, Las Vegas, NV, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Discussion

The measurement of toxic compounds in the atmosphere is simplified by the fact that each compound has a specific spectral "fingerprint." The identification of the various "fingerprints," or compounds, can be routine by FT-IR. The measurement can be made on the site,

or, should the situation necessitate it, at a reasonable distance downwind from the site.

The sensitivity and selectivity of FT-IR methods for volatile organics is excellent for low resolution spectroscopy and is fully expected to be so for high resolution. However, the speed and economics relative to conventional air-toxic methods merits further scrutiny, and Table 1 compares the analysis time of the two techniques. In addition to the advantage of producing near real-time data, a major advantage of the long-path FT-IR approach over point sample collection/analysis techniques is the cost effectiveness. Most air pathway analyses (APA) at Superfund sites use the point sampling approach in spite of the dynamic nature of air masses. Many samples are collected and analyzed to compensate for this temporal variability but not without a considerable expenditure of time and money (\$500-1000/sample).

This study has demonstrated that this FT-IR system can be used to detect toxic compounds in the atmosphere over a Superfund site. Within a matter of hours after the van arrives on a site, qualitative and quantitative information on toxic atmospheric compounds can be available. From this information one can make recommendations for additional monitoring studies, removal or remedial action, and determine if pre-established safety levels are being exceeded. This mobile laboratory enhances the capability of present and future site assessment.

Performance of the spectrometer is presented in Table 2. The table provides wave numbers of peaks used for

Table 1. Comparison of Analysis Times per Canister and for Open-Path Infrared Methods^a

	Sample Collection Time, Hrs	Cryofocus Desorption, Mins	Instrument Time, Mins	Minimum-Maximum Time, Mins
Canister	0-24 ^b	10-30	45	25-80
FT-IR	0	0	5-60 ^c	5-60

^a Multiple canister analyses are required to profile a field site.

^b To completely fill canister. Zero indicates almost instantaneous sample collection.

^c Dependent on ambient pollutant concentrations, spectral complexity, and operator skill.

identification and quantitative determination of volatile organics, the spectral resolution obtained in the transformed spectra, and the detection limit for most compounds at a path length of 100 meters. The compounds include a variety of purgable halogen containing compounds and purgable aromatics measured by current EPA methods, as well as non-purgables (e.g., n-butanol, 1,4-dioxane and ethyl acetate) not amenable to standard methods.

Table 2. Estimated Detection Limits (ppb) for Some Volatile Organic Compounds (VOCs) at a Path Length of 100 Meters Using an Appropriate Absorption Band from the Mid-Infrared Region

Compound	Wavenumber (cm^{-1})	Resolution (cm^{-1})	Detection Limit (ppb) ^a
<i>Chlorinated hydrocarbons</i>			
Allyl chloride	756.9	0.5	67
Carbon tetrachloride	795.2	0.5	6.3
Chlorobenzene	741.2	0.1	26
Chloroform	772.6	0.5	b
1,2-Dichloroethane	731.3	0.5	34
Methylene chloride	749.5	0.5	20
Tetrachloroethylene	916.3	0.5	19
1,1,1-Trichloroethane	726.3	0.5	8.1
Trichloroethylene	849.4	0.5	18
<i>Aromatic hydrocarbons</i>			
Benzene	673.9	0.1	c
Ethylbenzene	2794.0	0.5	31
Pyridine	700.3	0.1	c
Toluene	694.3	0.1	c
<i>Alkane</i>			
Cyclopentane	2966.0	0.5	7.2
<i>Alcohols</i>			
<i>n</i> -Butanol	2967.4	0.5	22.4
	1068.8	0.5	35
Ethanol	1066.1	0.5	31
Isopropanol	2982.7	0.5	19
	956.5	0.5	76
Methanol	1033.4	0.1	18
	1033.4	0.5	8.1
<i>Ketones</i>			
Acetone	1217.7	0.5	36
Methyl ethyl ketone	1174.2	0.5	40
Methyl isobutyl ketone	2965.4	0.5	18
<i>Ester</i>			
Ethyl acetate	1241.4	0.5	5.0
<i>Ethers</i>			
Diethyl ether	1142.9	0.5	9.3
1,4-Dioxane	2863.1	0.5	11
	1138.3	0.5	9.9
Tetrahydrofuran	2981.7	0.5	17
	1084.4	0.5	26

^a These detection limits, using concentration in parts per billion (ppb), are for P = 740 torr and T = 298 K.

^b These measurements are being repeated.

^c These bands fall in spectral regions containing sharp water vapor absorption bands, and the detection limits are dependent on humidity.

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The complete report, entitled "Field Demonstration for Mobile FT-IR for Detection of Volatile Organic Chemicals," (Order No. PB 90-192 014/AS; Cost: \$23.00, subject to change) will be available only from:

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