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Air



Asphalt Roofing Industry Fourier Transform Infrared Spectroscopy Modified Bitumen

U.S. Intec
Port Arthur, Texas



Emissions Test at an Asphaltic Roofing Manufacturer

Test Report

U.S. Intec, Inc.
Port Arthur, Texas

Prepared for
U.S. Environmental Protection Agency

Office of Air Quality Planning and Standards
Emissions, Monitoring and Analysis Division
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PREFACE

This test report was prepared by Midwest Research Institute (MRI) for the U. S. Environmental Protection Agency (EPA) under EPA Contract No. 68D-98-027, Work Assignment No. 2-11. Mr. Michael Toney is the EPA Work Assignment Manager (WAM). Dr. Thomas Geyer is the MRI Work Assignment Leader (WAL). The field test was performed under EPA Contract No. 68-D2-0165, Work Assignment No. 4-21. A draft report was prepared under EPA Contract No. 68-W6-0048, Work Assignment No. 2-08. Mr. Toney was also the WAM for the previous work assignments. Dr. Geyer was the MRI WAL for Work Assignment No. 4-21 and the Task Leader for Work Assignment No. 2-08. Mr. John Hosenfeld was the MRI WAL for Work Assignment No. 2-08.

MIDWEST RESEARCH INSTITUTE


for John Hosenfeld
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1.0 INTRODUCTION

1.1 BACKGROUND

A "Request for Emissions Testing at Four Asphalt Roofing and Processing Facilities" was submitted by the U.S. EPA Emission Standards Division (ESD), Minerals and Inorganic Chemicals Group (MICG) to the Emission Measurement Center (EMC). The Emission Measurement Center directed Midwest Research Institute (MRI) to conduct emissions testing at asphalt roofing plants. This report presents results of MRI's FTIR and Method 25A testing conducted at U. S. Intec in Port Arthur, Texas. The field measurements were performed in September 1997 under several test conditions for both controlled and uncontrolled emissions.

1.2 PROJECT SUMMARY

The purpose of this test program was to obtain uncontrolled and controlled HAP emissions data from asphalt roofing and processing plants to support a national emission standard for hazardous air pollutants. Specifically, the objective was to measure HAPs in several processes. An additional goal was to measure other compounds that could be detected with the FTIR system.

Emissions were measured at both the inlet and outlet of the incinerator (thermal oxidizer) used to control emissions from mixing and holding tanks. Additionally, uncontrolled emissions from individual mixing and holding tanks and coaters were measured. A total of eight sampling locations were tested, noted as E1 through E8 in Table 1. Midwest Research conducted FTIR testing using EPA Method 320, and hydrocarbon testing using EPA Method 25A. Eastern Research Group, Inc. (ERG) performed manual methods at the thermal oxidizer inlet and outlet. Table 1 shows the test matrix and summarizes the tests performed for MRI's portion of the field testing.

Three test runs were conducted by alternating sampling at the inlet and outlet of the thermal oxidizer. The sampling time for the FTIR and THC methods (approximately 4 hr per run) coincided with ERG's manual sampling periods.

Similarly, the two coater vents (roof stacks) for both the SBS and APP product lines were tested during three separate runs each (approximately 1 hr each). Finally, one test run each (approximately 1 hr) was conducted on both the holding and mixing tanks for both the APP and SBS product lines.

TABLE 1. TEST MATRIX

Date	Emission point	Description	Sampling location	Sample type	Sampling method	No. of test runs	Duration
9/22 9/23	E1	Holding and Mixing Tank Collection Header	Thermal Oxidizer Inlet	THC All Gaseous HAP	Method 25A FTIR	3	4 hr, performed simultaneous with outlet test runs
9/22 9/23	E2	Holding and Mixing Tank Collection Header	Thermal Oxidizer Outlet	THC All Gaseous HAP	Method 25A FTIR	3	4 hr, performed simultaneous with inlet test runs
9/26	E3	Modified Bitumen Holding Tank	Tank Outlet (SBS Tank 3)	THC All Gaseous HAP Flow	Method 25A FTIR Methods 1-2	1	1 hr
9/26	E4	Modified Bitumen Holding Tank	Tank Outlet (APP Tank 1)	THC All Gaseous HAP Flow	Method 25A FTIR Methods 1-2	2 ^a	1 hr
9/25	E5	Modified Bitumen Mixing Tank	Tank Outlet (SBS Tank 11)	THC All Gaseous HAP	Method 25A FTIR	1	1 hr
9/25	E6	Modified Bitumen Mixing Tank	Tank Outlet (APP Tank 1)	THC All Gaseous HAP	Method 25A FTIR	1	1 hr
9/24/97	E7	Coater	Roof Stack Outlet (APP)	THC All Gaseous HAP	Method 25A FTIR	3	1 hr
9/24 & 9/25	E8	Coater	Roof Stack Outlet (SBS)	THC All Gaseous HAP	Method 25A FTIR	3	1 hr

^a One test was performed but repeated due to sampling problems, for a total of two test runs.

1.3 KEY PROJECT PERSONNEL

A list of the key project personnel, their organization, title, and phone numbers are presented in Table 2.

TABLE 2. PROJECT PERSONNEL

Organization and Title	Name	Phone No.
U.S. Intec Project Engineer	Jeff Hughes	(409) 724-7024
U. S. EPA, EMC Work Assignment Manager	Michael L. Toney	(919) 541-5247
MRI Work Assignment Leader Contract No. 68-W6-0048, Work Assignment No. 2-08	John Hosenfeld	(816) 753-7600, ext 1336
MRI Work Assignment Leader Contract No. 68-D2-0165, Work Assignment No. 4-21 Contract No. 68D-98-027 Work Assignment 2-11	Thomas J. Geyer	(919) 851-8181, ext 3120

2.0 PROCESS DESCRIPTION AND TEST LOCATIONS

The U.S. Intec facility in Port Arthur, Texas, was selected as a test site representative of the modified bitumen production process in the asphalt roofing industry. The site uses the modified bitumen process using atactic polypropylene (APP) or styrene-butadiene-styrene (SBS).

2.1 PROCESS DESCRIPTION

The facility produces rolled roofing products by saturating a polyester substrate and a fiberglass substrate with modified bitumen in two separate production lines (APP or SBS). A flow diagram of the process is included in Figures 1 and 2. Sampling points, as noted earlier in Table 1, are designated as E1 through E8. Both the APP and SBS substrates enter their respective production lines through a web unwind stand and then go through a dry looper. Asphalt is unloaded from tanker trucks into two 100-ton, 350°F asphalt storage tanks. Asphalt from the storage tanks is distributed to six 10.5-ton, 400°F mixing tanks for the production line using polyester substrate and two 10.5-ton, 390°F mixing tanks for the production line using fiberglass substrate. Tanker trucks also unload polymer liquid into two steam-jacket storage tanks.

Modified bitumen is produced by combining the asphalt with polypropylene and fillers in the six mixing tanks for the line using polyester substrate. Modified bitumen is produced for the line using fiberglass substrate by combining asphalt with SBS in one mixing tank and fillers in the second mixing tank. The modified bitumen in the mixing tanks is transferred to two holding tanks for the line using polyester substrate and one holding tank for the line using fiberglass substrate before going to the respective coaters. The coaters are impregnation vats where the substrates are saturated with the modified bitumen. Once the saturated polyester substrate leaves the vat, it is coated with granules and talc. The saturated fiberglass substrate is coated with granules and sand. After both products are cooled, they go through separate finish loopers and roll winders.

The facility operates 24 hr per day from Monday morning through Friday evening (5 days per week).

2.2 CONTROL EQUIPMENT DESCRIPTION

Emissions from the holding and mixing tanks for both SBS and APP production lines are ducted to the thermal oxidizer. The gas stream passes through a booster fan to a cyclone

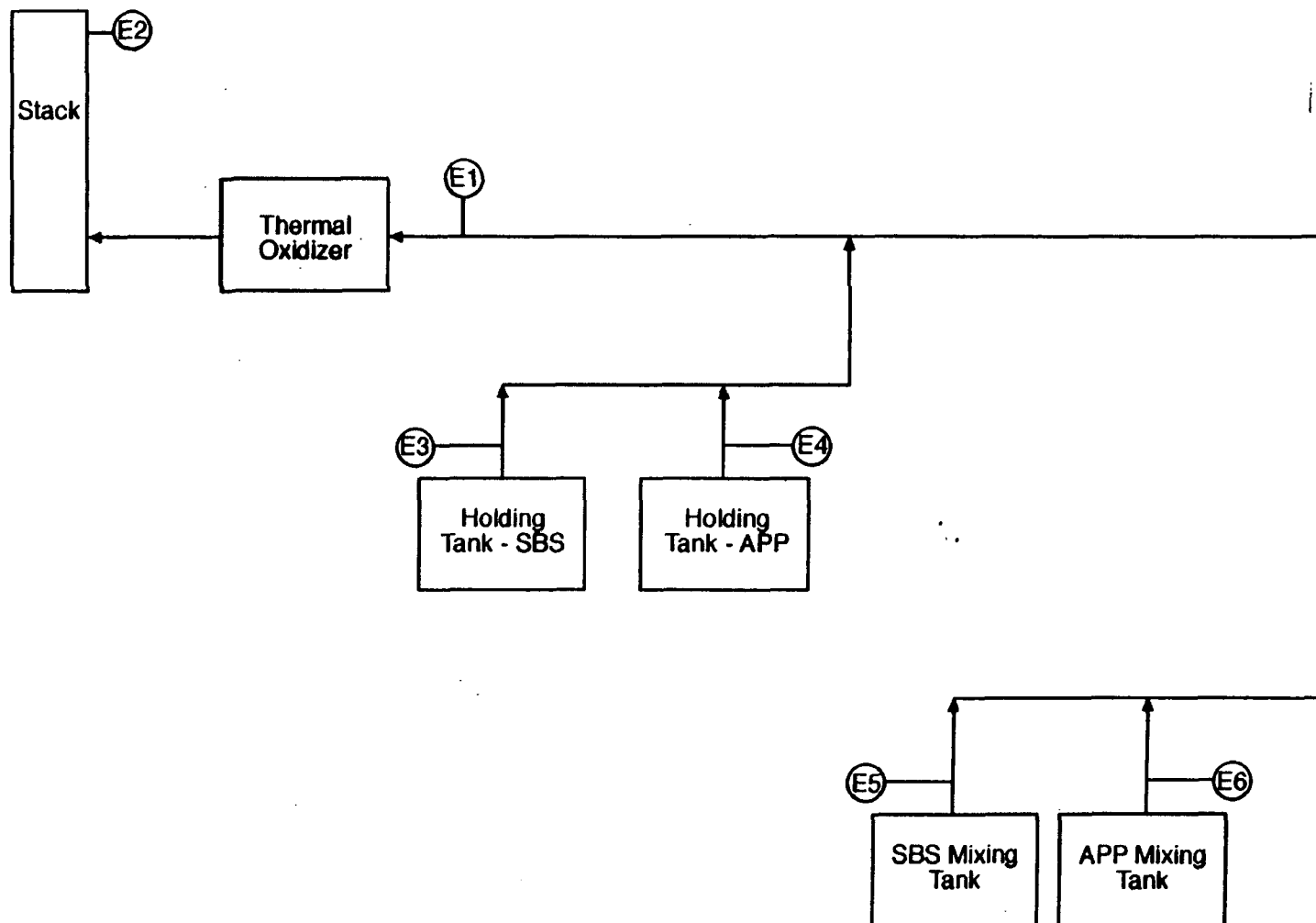


Figure 1. Modified bitumen operations--U.S. Intec, Inc., Port Arthur, Texas.

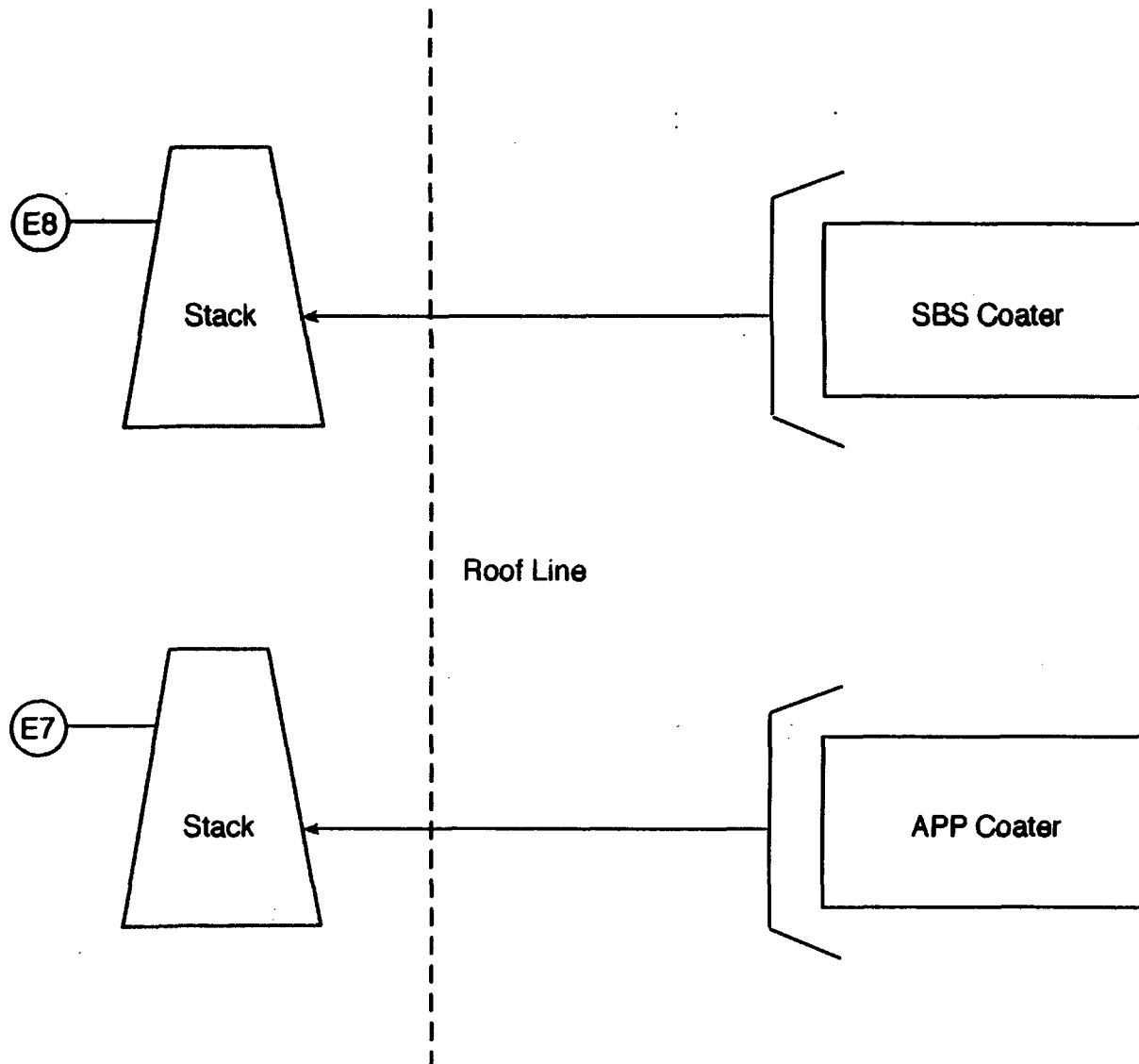


Figure 2. Coater operations--U.S. Intec, Inc., Port Arthur, Texas.

separator where coarse particulate matter is removed. The thermal oxidizer operated at a temperature of 1400°F and a residence time of 0.5 seconds. Gas was moved from the thermal oxidizer to the stack by an induced draft fan where gas temperatures were approximately 480°F, at a nominal flow rate of 10,000 acfm (23.6 ft/sec velocity).

Emissions from holding and mixing tanks were not controlled at the locations tested, and the coaters are not controlled, but vent to the atmosphere. Gas stream temperatures from the mixing and holding tank outlet ducts ranged from 110° to 316°F at pressures slightly less than atmospheric pressure. Velocity heads in these ducts were very low and required measurement with a hot wire anemometer. Gas streams in the coater vent stacks had temperatures of approximately 90° to 110°F and pressures above atmospheric pressure (an in of water or more). Velocity heads in these ducts were approximately 0.60 in of water, or greater.

The water vapor content at all sampling locations except the thermal oxidizer outlet stack was close to ambient conditions. The water vapor content in the thermal oxidizer outlet stack was approximately 4 percent to 7 percent by volume.

2.3 SAMPLING AND MONITORING LOCATIONS

Sampling was conducted at a total of 8 different locations, noted previously as locations E1 through E8 in Table 1 and Figures 1 and 2. Each of the following sections briefly describes the sampling locations in greater detail. Sections 2.3.1 and 2.3.2 describe the inlet and outlet locations for the thermal oxidizer, which is fed via a common duct. Sections 2.3.3 and 2.3.4 describe exhaust ducts from the individual holding tanks which feed into the common duct. Sections 2.3.5 and 2.3.6 describe exhaust ducts from the individual mixing tanks which feed into the common duct. Sections 2.3.7 and 2.3.8 describe vent stacks for the coating processes, which are not part of the thermal oxidizer treatment system.

2.3.1 Thermal Oxidizer Inlet Duct (E1)

Thermal oxidizer inlet sampling was conducted in the common manifold (header) which collects emissions exhausted from the mixing and holding tanks from both production lines. A schematic drawing of the inlet sampling location is presented in Figure 3. Two 4-in ports (nipples), 90° apart, were installed in cross-section (CS) 2 of the horizontal, circular, steel duct for ERG's sampling and velocity traverses. A 3-in port (nipple) was installed in CS1 for the Method 25A and 320 (FTIR) single-point sampling. Temporary scaffolding for access from the

ground to the location was installed. Approximately 150 ft of sample transfer line from the trailer was required here.

2.3.2 Thermal Oxidizer Outlet Stack (E2)

Thermal oxidizer outlet sampling was conducted in the stack immediately downstream of the thermal oxidizer. The outlet sampling location, approximately 30 ft above ground level, is also presented in Figure 3. The two existing 3-in ports, 90° apart, in CS4 of the circular, steel stack were replaced with 4-in nipples and were used for ERG's sampling and velocity traverses. A 3-in port (nipple) was installed in CS3 for the Method 25A and 320 (FTIR) single-point sampling. Approximately 200 ft of sample transfer line from the trailer was required here.

2.3.3 Modified Bitumen Holding Tank Exhaust Outlet E19B (E3)

This sampling location is in a horizontal run of 10-in diameter steel duct (E19B) exhausting emissions from SBS production line holding tank No. H3. One 3-in port was installed on the side of the duct at a location directly over holding tank No. H1. The duct is approximately 30 ft above the production room floor, just below the roof. The top of the tank is accessible by stairs from the production room floor and a walkway. Approximately 200 ft of sample transfer line from the trailer were required here. Only one diameter was traversed for volumetric flow rate measurements because velocities were very low and stratification across the gas stream was insignificant. Appendix A contains traverse point information and a sketch of the sampling port arrangement for this location.

2.3.4 Modified Bitumen Holding Tank Exhaust Outlet E1B (E4)

This sampling location was a vertical section of 8-in diameter black iron pipe (E1B) exhausting emissions from APP production line holding tank No. H1. The duct was right off the top of the tank and was accessible from a permanent platform on top of the tank. One 3-in port was installed on the side of the duct at a location such that the sampling equipment was just outside of the handrails and supported from an overhead beam. This location was approximately 20 ft above the production room floor and accessible by stairs from the production room floor and a walkway. Approximately 200 ft of sample transfer line from the trailer were required here. Again, only one diameter was traversed for volumetric flow rate measurements because velocities were very low and stratification across the gas stream was insignificant. Appendix A

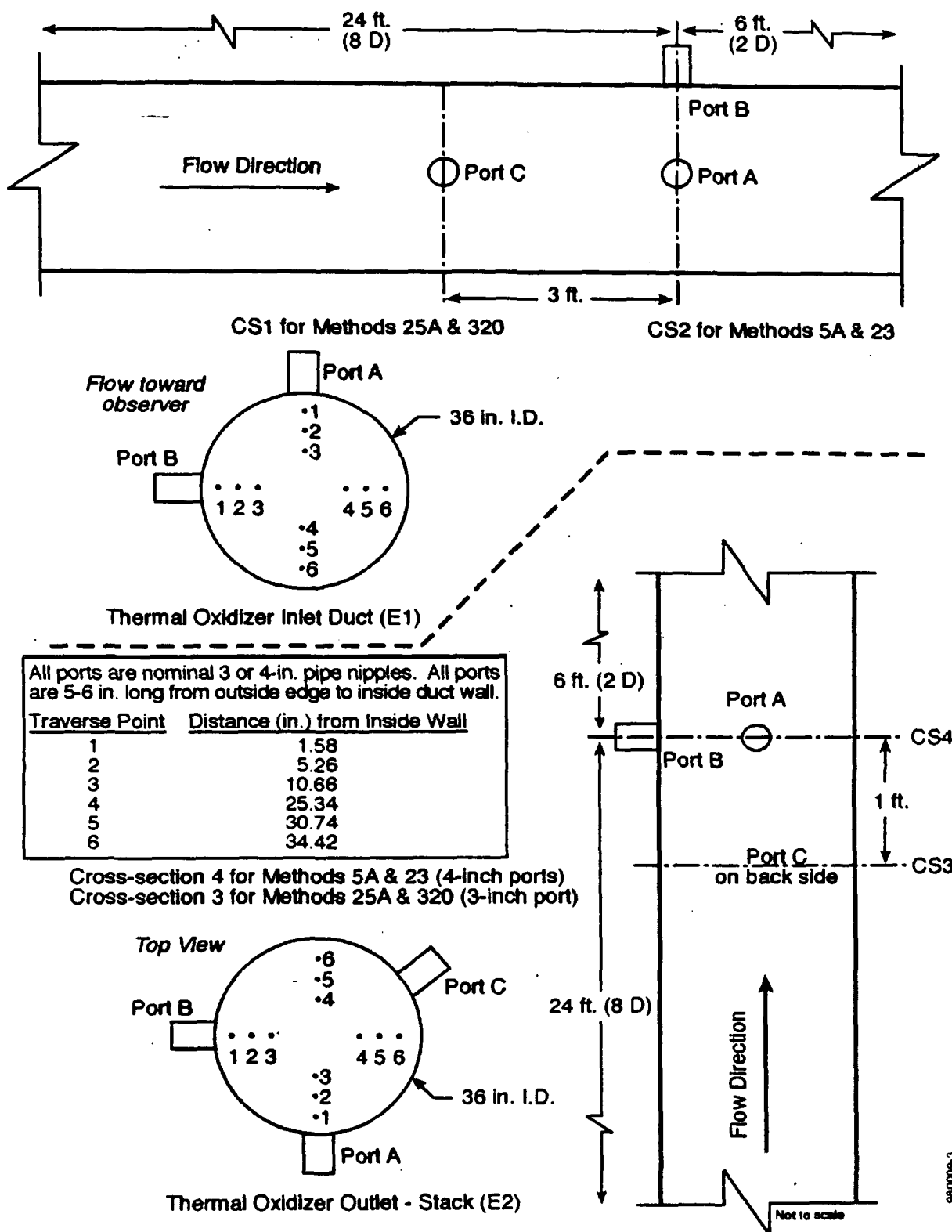


Figure 3. Thermal oxidizer inlet and outlet sampling location.

contains traverse point information and a sketch of the sampling port arrangement for this location.

2.3.5 Modified Bitumen Mixing Tank Exhaust Outlet E17B (E5)

This sampling location was a horizontal section of 8-in diameter steel duct (E17B) exhausting emissions from SBS production line mixing tank No. M7. The duct was approximately 12 ft above floor level. This floor level was accessible by stairs from the ground level. One 3-in port was installed on the side of the duct. Approximately 100 ft of sample transfer line from the trailer was required here. Only one diameter was traversed for volumetric flow rate measurements because velocities were very low and stratification across the gas stream was insignificant. Appendix A contains traverse point information and a sketch of the sampling port arrangement for this location.

2.3.6 Modified Bitumen Mixing Tank Exhaust Outlet E2B (E6)

This sampling location was a horizontal section of 8-in diameter steel duct (E2B) exhausting emissions from APP production line mixing tank No. M1. The duct was approximately 10 ft above floor level. This location was above the production room floor and was accessible by stairs from the production room floor and a walkway. One 3-in port was installed on the side of the duct. Approximately 200 ft of sample transfer line from the trailer were required here. Only one diameter was traversed for volumetric flow rate measurements because velocities were very low and stratification across the gas stream was insignificant. Appendix A contains traverse point information and a sketch of the sampling port arrangement for this location.

2.3.7 Coater Vent Stack E10S (E7)

This sampling location was a vertical, 29-in I.D. steel duct or "stack" (E10S) exhausting emissions from APP coater vat No. L3. The duct was located on the slanted, metal sheet roof (closest stack to the access ladder up the side of the building). Two 2-in ports, 90° apart, were about 5 ft above the roof. These ports were replaced with 4-in ports (nipples) for ERG's sampling and velocity traverses. Another 4-in port was installed 1 ft below and offset 45° from the other ports for the Method 25A and 320 (FTIR) single-point sampling. Approximately 200 ft of sample transfer line from the trailer were required here. Appendix A contains traverse point information and a sketch of the sampling port arrangement for this location.

2.3.8 Coater Vent Stack E20S (E8)

This sampling location was a vertical, 29-in I.D. steel duct or "stack" (E20S) exhausting emissions from SBS coater vat No. L9. The duct was located approximately 50 ft further up the roof from location E7. Otherwise, all information described above in Section 3.7 also applies to this location. Appendix A contains traverse point information and a sketch of the sampling port arrangement for this location.

3.0 RESULTS

3.1 SCHEDULE

Testing of the U.S. Intec, Inc. facility in Port Arthur, Texas, was performed from September 22-26, 1997. Table 1 summarizes the schedule and the specific tests performed. Sampling logs and notes for the Method 25A (THC) and Method 320 (FTIR) sampling are contained in Appendix D. The THC and FTIR sampling was performed in coordination with the manual sampling conducted by ERG.

3.2 FIELD TEST PROBLEMS AND CHANGES

Several deviations from the Test Plan were performed to adapt to field conditions. The following is a summary of these changes.

1. Difficulties with one of the THC analyzers prevented the simultaneous operation of both analyzers. Therefore, inlet/Outlet testing of the thermal oxidizer was accomplished by sampling in alternating 30-min intervals at either location using a single THC analyzer. In order to provide a parallel data set, the FTIR sampled the same location as the single THC analyzer, and alternated between locations on the same 30-min schedule.
2. An additional problem with the THC data logging system necessitated manual data logging during Run 1. For all of the remaining tests a computerized data logger was used.
3. At the request of EPA representatives on site, the 2-hr sampling period for the inlet/outlet testing of the thermal oxidizer was extended to 4hrs. All three of the thermal oxidizer tests were 4 hr.
4. Due to sampling error, ambient air was drawn into the sampling system during Run 1 on the APP Holding Tank 1. This test was repeated and no 25A analysis of the Run 1 APP Holding Tank 1 data was performed.
5. During the final test, Run 2 on the APP Holding Tank 1, particulate buildup in the sampling lines caused failure of the heated pumps. As a consequence, the FTIR sampling was changed from continuous spectral collection to batch collection, and was performed manually. For each batch sample, the cell was flushed twice with dry nitrogen, evacuated, then filled with sample gas.
6. Absorbance bands were much greater than 1 in the analytical region near 2900 cm^{-1} in some spectra from Run 1 at the APP mixing tank and Run 2 at the APP holding tank. At these locations some spectra of diluted samples were recorded to bring the entire spectrum on-scale. The dilution procedure involved removing some sample from the gas cell, noting the sample pressure and then filling the cell with dry nitrogen to ambient pressure. The spectrum of the static, diluted sample was then recorded. The readings from the Barocell pressure gauge were used to determine an approximate a dilution ratio. The dilution ratios were included in the concentration calculations.
7. Samples were spiked in two different ways. For the first day, a blended gas containing both SF_6 and a volatile target compound was not available, requiring two separate gases to be blended through two mass flow controllers and then spiked into the sample lines. Spiking after the first day was performed using a single blended gas containing both SF_6 and

- p*-xylene as the target volatile organic. Since all locations were spiked with the *p*-xylene/SF₆ mixture, these results are reported in the spike summary.
8. Because of concern about interference from high CO₂ concentrations, the analyte spike of the *p*-xylene gas standard was controlled at a flow rate of approximately 2.0 Lpm with a dilution ratio of about 5:1. Much lower spike flow rates were used at the coater roof stacks.
 9. Due to time restrictions in coordinating testing with ongoing plant operations, spiking during the first four sampling days was performed in duplicate, rather than in triplicate. Triplicate spiking was performed on the last day.
 10. Spectra collected during the last two days occasionally contained especially high concentrations of hydrocarbon species. Some of the hydrocarbons may have adhered to the cell walls in subsequent samples, but this had little or no effect on the analytical results. Some additional nitrogen background spectra were recorded to minimize this effect.
 11. A second post-run CTS spectrum was not recorded on 9/22/97. However, the Initial CTS spectra from 9/22/97 and 9/23/97 past the method criteria. Therefore, the first CTS spectrum on 9/23 also serves as the post-run CTS for the run on 9/22/97. The average deviation of all the CTS measurements from their average value was 2.8 percent.
 12. The FTIR cell did not pass the vacuum leak check during the field test (leak <4 percent of cell volume according to the EPA protocol). Gas was sampled continuously, whenever practical, to avoid diluting the sample. When continuous sampling was not practical, the cell was filled above ambient pressure and the sample spectrum was recorded when the cell pressure reached equilibrium. A leak would result in a low bias in the reported concentrations, but the sampling procedures used should have minimized any effect on the results.

3.3 FTIR RESULTS

A summary of the quantitative FTIR results and the average mass emissions rates is given in Table 3. Complete tables of FTIR results are in Appendix E.

TABLE 3. SUMMARY OF FTIR RESULTS AND MASS EMISSIONS RATES

Location	Benzene			Carbonyl sulfide			Methyl chloroform			Ethylidene dichloride			Methanol		
	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr
TO Inlet				0.035	2.7E-03	1.2E-03									
Run 1				0.000	0.000	0.000									
Run 2				0.0054	3.9E-04	1.8E-04									
Run 3															
TO Outlet				0.000	0.000	0.000									
Run 1				0.000	0.000	0.000									
Run 2				0.000	0.000	0.000									
Run 3				0.000	0.000	0.000									
APP Coater															
Run 1															
SBS Coater															
Run 1															
APP Mixing Tank				0.74	5.1E-05	2.3E-05							0.14	5.2E-06	2.4E-06
Run 1															
SBS Mixing Tank				0.024	9.6E-06	4.4E-06									
Run 1															
APP Holding Tank	65.9	7.4E-02	3.4E-02	1.6	1.4E-03	6.3E-04				9.5	1.8E-02	8.3E-03	0.063	2.9E-05	1.3E-05
Run 1															
SBS Holding Tank				0.73	2.1E-04	9.4E-05	0.46	2.9E-04	1.3E-04				0.0078	1.2E-06	5.4E-07
Run 1															

Location	Styrene			1,1,2,2-Tetrachloroethane			p-Xylene			2,2,4-Trimethylpentane			Ethylene		
	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr
TO Inlet							0.21	0.028	0.013	0.44	0.064	0.029	0.000	0.000	0.000
Run 1							0.000	0.000	0.000	0.000	0.000	0.000	0.0027	9.0E-05	4.1E-05
Run 2							0.052	6.6E-03	3.0E-03	0.000	0.000	0.000	0.19	6.5E-03	2.9E-03
Run 3															
TO Outlet							2.0	0.26	0.12	0.050	7.1E-03	3.2E-03	0.000	0.000	0.000
Run 1							0.000	0.000	0.000	0.000	0.000	0.000	0.0094	3.2E-04	1.4E-04
Run 2							2.8	0.35	0.16	0.000	0.000	0.000	0.016	5.2E-04	2.4E-04
Run 3															
APP Coater															
Run 1															
SBS Coater															
Run 1															
APP Mixing Tank													1.5	4.7E-05	2.2E-05
Run 1															
SBS Mixing Tank															
Run 1															
APP Holding Tank															
Run 1															
SBS Holding Tank	1.1	5.4E-04	2.4E-04	0.32	2.6E-04	1.2E-04	1.1	5.5E-04	2.5E-04						
Run 1															

TABLE 3. (continued)

Location	Propane			Cumene			Hexane			Methylene chloride			Propionaldehyde		
	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr
TO Inlet															
Run 1	3.5	0.20	0.089	1.2	0.18	0.083	11.0	1.19	0.54						
Run 2	3.5	0.19	0.084	5.1	0.74	0.34	11.3	1.17	0.53						
Run 3	4.2	0.22	0.099	6.1	0.88	0.40	11.4	1.17	0.53						
TO Outlet															
Run 1	0.48	0.026	0.012	0.08	0.013	5.7E-03	1.5	0.16	0.07						
Run 2	0.24	0.013	5.9E-03	0.08	0.011	0.005	0.85	0.088	0.040						
Run 3	0.35	0.018	8.3E-03	0.20	0.028	0.013	0.45	0.046	0.021						
APP Coater Run 1							1.5	0.22	0.10						
SBS Coater Run 1							2.0	0.30	0.14						
APP Mixing Tank Run 1															
SBS Mixing Tank Run 1							38.4	0.022	9.8E-03						
APP Holding Tank Run 1							101.6	0.13	0.057				98.7	0.083	0.038
SBS Holding Tank Run 1	4.6	9.6E-04	4.3E-04				58.2	0.024	0.011	0.36	1.4E-04	6.5E-05	21.9	6.0E-03	2.7E-03

Location	Methane			Sulfur dioxide			Carbon monoxide			Ammonia			Formaldehyde		
	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr	ppm	lb/hr	kg/hr
TO Inlet															
Run 1	3.0	0.061	0.028				11.3	0.40	0.18				0.000	0.000	0.000
Run 2	3.0	0.058	0.026				0.22	7.4E-03	3.4E-03				0.000	0.000	0.000
Run 3	4.4	0.083	0.038				4.2	0.14	0.064				2.3	0.083	0.038
TO Outlet															
Run 1	0.36	7.2E-03	3.3E-03				1.3	0.043	0.020						
Run 2	0.16	3.0E-03	1.4E-03				0.17	5.6E-03	2.6E-03						
Run 3	0.40	7.7E-03	3.5E-03				0.18	6.2E-03	2.8E-03						
APP Coater Run 1	3.0	0.083	0.038				13.1	0.64	0.29						
SBS Coater Run 1	3.5	0.097	0.044				14.4	0.70	0.32						
APP Mixing Tank Run 1				6.6	4.8E-04	2.2E-04	58.4	1.9E-03	8.4E-04						
SBS Mixing Tank Run 1	4.3	4.5E-04	2.0E-04	77.0	0.032	0.015	9.1	1.7E-03	7.5E-04	4.0	4.4E-04	2.0E-04			
APP Holding Tank Run 1				109.6	0.10	0.046	143.2	0.058	0.026	10.8	2.7E-03	1.2E-03	133.6	0.058	0.026
SBS Holding Tank Run 1	14.8	1.1E-03	5.1E-04	57.4	0.017	7.8E-03	118.7	0.016	7.1E-03	16.1	1.3E-03	5.8E-04	9.0	1.3E-03	5.8E-04

3.3.1 Thermal Oxidizer Inlet and Outlet

The results for the thermal oxidizer inlet and outlet are presented in Tables E-1 and E-2, respectively. Compound identifications and their concentrations result from a least-squares fit performed by the analytical program, using the available input data, which determined the best linear combination from the reference spectra in Section 4.5.1. The infrared absorbance near $3,000\text{ cm}^{-1}$ is primarily due to non-aromatic organic species. But the presence of cumene is consistent with the spectra because its strongest absorbance in this region is from the aliphatic hydrogens not from the aromatic (bonded to the ring) hydrogens. In the C-H stretching region (near $2,900\text{ cm}^{-1}$), hexane and trimethylpentane give the best fit of the organic HAPs included in the analysis.

3.3.2 APP and SBS Coaters

Emissions from the coater roof stacks were much lower compared to the other test locations. Table 4 presents results of uncertainty calculations for some HAP compounds. The results for the APP and SBS coater stacks are presented in Tables E-3 and E-4.

3.3.3 APP and SBS Mixing Tanks

Results from the APP and SBS mixing tanks are presented in Tables E-5 and E-6. Both locations exhibited high organic emissions. Portions of the spectra from the APP mixing tank were off scale and could not be quantified. Some compounds could not be measured because no quantitative reference spectra are available. These compounds are not included in Tables E-5 and E-6. These other emissions include propylene and isomers of pentene. These emissions could be quantified if quantitative reference spectra of each compound were first measured in the laboratory. The additional reference spectra could then be included in the analytical computer program. Table 5 shows some additional compounds that may be included in the emissions, but cannot be measured because there are no quantitative reference spectra available.

3.3.4 APP and SBS Holding Tanks

Results from the APP and SBS holding tanks are presented in Tables E-7 and E-8. Significant organic emissions, carbonyl sulfide, CO and ammonia were detected at each location. Some compounds are identified in Tables E-7 and E-8. Additional organic compounds that were not measured may include propylene and pentene compounds.

**TABLE 4. UNCERTAINTY RESULTS FOR SOME HAP COMPOUNDS
AT THE COATER STACKS**

HAP-name	Uncertainty, ppm	
	APP coater	SBS coater
Benzene	1.191	0.883
Carbonyl Sulfide	0.088	0.066
Methyl chloride	4.063	3.013
Methyl chloroform	0.081	0.066
1,1-Dichloroethane	0.450	0.367
Toluene	3.981	2.952
1,3-Butadiene	0.350	0.292
Propane	0.773	0.574
Cumene	1.465	1.087
Ethyl benzene	4.280	3.174
Methylene Chloride	0.183	0.149
Propionaldehyde	0.823	0.610
Styrene	0.595	0.485
1,1,2,2-Tetrachloroethane	0.265	0.216
p-Xylene	0.578	0.471
o-Xylene	2.252	1.670
m-Xylene	3.114	2.309
2,2,4-Trimethylpentane	0.360	0.267
Formaldehyde	0.572	0.424

TABLE 5. POSSIBLE DETECTS OF SOME ORGANIC SPECIES

Compound	APP Holding Tank 1	SBS Holding Tank 3	SBS Mixing Tank 1	APP Mixing Tank 1
3-methyl,1-butene				1
2-methyl,1-pentene	1	1	1	
Propylene	2	2		
Propane	1	1		1
2-pentene	1	1		1
4-methyl,2-pentene	1	1		1
pentane	1	1		

1 - Indicates a possible detect. This list is not exhaustive.

2- Indicates a certain detect.

3.3.5 Results from Spiked Samples

Some samples were spiked with a controlled flow containing a mixture of *p*-xylene and SF₆. The SF₆ was used to determine the spike dilution factor. The SF₆ and *p*-xylene concentrations were determined with the same analysis program that was used for the other analyses. The spike results are summarized in Table 6. Explanations of the calculations are given in the footnotes to Table 6 and in Section 4.4.

Two spike recoveries are presented in Table 6. The recoveries in column A result from using the *p*-xylene reference spectra in the EPA spectral library. Spectra of the *p*-xylene cylinder standard disagree with the EPA library spectra by about 25 percent. These spectra give the recovery results shown in column B of Table 6. In this test the spike recoveries fall within the requirement of ± 30 percent whichever reference data set is used.

The discrepancy between the library spectra and the spectra of the cylinder standard is illustrated in Table 7. This table compares the integrated absorbance band areas for the spectra after correction for differences in temperature and pathlength. The same table also compares the spectra based on their accepted concentrations after correction for differences in temperature and path length. Ideally the two comparisons would agree. In this case they differ by about 25 percent. The results from the analytical program depend on the absorbance values of the reference spectra so this discrepancy affects the analytical results. This observation is compound dependent and nothing can be inferred about the reported results for other compounds.

TABLE 6. SUMMARY OF ASPHALT ROOFING FTIR P-XYLENE SPIKE RESULTS

Location	Date	Average p-xylene concentration			Average SF ₆ concentration			DF	Cexp	Δ	% Recovery	
		Spike	Unspike	Calc	Spike	Unspike	Calc				A	B
Thermal Oxidizer Inlet	9/23/97	29.9	0.0	29.9	0.939	0.000	0.939	4.3	23.9	6.0	125.0	93.3
	9/23/97	28.3	0.0	28.3	0.895	0.000	0.895	4.6	22.8	5.5	124.1	92.6
Thermal Oxidizer Outlet	9/23/97	24.4	0.0	24.4	0.742	0.000	0.742	5.5	18.9	5.5	129.1	96.3
APP Coater	9/24/97	7.6	0.0	7.6	0.259	0.000	0.259	15.7	6.6	1.0	115.3	86.0
SBS Coater Roof Stack	9/24/97	10.7	0.0	10.7	0.324	0.000	0.324	12.6	8.2	2.5	129.7	96.8
	9/25/97	25.1	0.0	25.1	0.823	0.000	0.823	5.0	21.0	4.2	119.9	89.4
SBS Mixing Tank 11	9/25/97	23.3	0.0	23.3	0.856	0.000	0.856	4.8	21.8	1.5	107.0	79.8
SBS Holding Tank 3	9/26/97	21.9	3.1	18.8	0.618	0.000	0.618	6.6	15.7	3.0	119.1	88.9
APP Holding Tank 1	9/26/97	30.4	0.0	30.4	0.975	0.000	0.975	4.2	24.9	5.5	122.1	91.1

"Spike" is the measured concentration of p-xylene or SF₆ in the spiked samples. "Unspike" is the measured concentration of p-xylene or SF₆ in the unspiked samples. Calc is the difference, spike - unspike. DF is the dilution factor, 4.08 ppm/SF₆(Calc). Cexp is the expected p-xylene concentration (104 ppm/DF). Δ is the difference, p-xylene (Calc) - Cexp. The % Recovery of 104 ppm p-xylene standard is relative to the EPA library spectra, column A, relative to spectra of the p-xylene calibration standard measured while at the Port Arthur test site, column B.

TABLE 7. p-XYLENE SPECTRAL BAND AREAS. COMPARISON OF EPA LIBRARY SPECTRA TO SPECTRA OF P-XYLENE CYLINDER STANDARD

p-xylene spectra	Source	Band area	Region, cm-1	Spectra comparison based on band areas		Comparison of spectra based on standard concentrations			
				Ratio (Ra)	=1/Ra	(ppm-m)/K	Ratio (Rc)	=1/Rc	Ra/Rc, %
173a4asa (1cm-1)	EPA library	6.5	818.6 - 769.9	5.5	0.182	5.05	5.1	0.197	92.45
173a4asc (1cm-1)		1.2		1.0	1.000	1.00	1.0	1.000	100.40
Dir03	Port Arthur	3.1	818.6 - 769.9	2.6	0.387	2.00	2.0	0.500	77.5
Dir04		3.3		2.7	0.364	2.00	2.0	0.500	72.8
Dir05		3.3		2.8	0.364	2.00	2.0	0.500	72.8

3.4 METHOD 25A RESULTS

THC results as determined by EPA Method 25A are presented in Tables 8 to 10. Appendix B contains the raw data and graphical displays of the data versus time.

As shown in Table 8, THC emissions from the outlet of the thermal oxidizer averaged near 2 ppm as propane (wet). Run 1 emissions were the highest of the three runs, but were collected by manually logging the data. The Run 1 manual readings likely introduced a high bias, since all the readings fell near the extreme low end (zero point) of the instruments scale, 0 to 1,000 ppm as propane. Runs 2 and 3 were electronically logged and are believed to be more accurate.

The THC concentrations at the inlet to the thermal oxidizer ranged from 60 to 100 ppm as propane (wet), with an average concentration of about 75 ppm. Concentrations were fairly stable, with an occasional spike of 5 to 10 ppm above the average being observed. Only once was a spike greater than 10 ppm above the average observed.

Mass emission rates of THC (in carbon equivalents) ranged from 3.1 to 3.5 lb/hr (Thermal Oxidizer Inlet) to 0.0043 to 0.0086 lb/hr (Thermal Oxidizer Outlet). The calculated mass emission rate of 0.279 lb/hr for Run 1 of the Thermal Oxidizer Outlet is nearly two orders of magnitude greater than either Runs 2 or 3, and further reinforces the believed inaccuracy of the manually logged data. Calculation of combustion efficiency, which is typically >99 percent for these types of combustion systems, also shows that Run 1 does not agree with Runs 2 and 3, and falls well below the expected 99 percent.

An examination of THC emissions from the SBS and APP Mixing and Holding Tanks (Table 9) shows that the APP line had much higher THC concentrations than the SBS line. For all the mixing and holding tanks tested, APP Mixing Tank 1 had the highest THC concentrations, and saw levels of 1,250 to 2,100 ppm. The APP Holding Tank 1 was next highest (475 to 875 ppm), followed by the SBS Mixing and Holding tanks, respectively (125 to 300 ppm).

In terms of THC mass emissions (in carbon equivalents), the APP line was also significantly greater than the SBS line. Due to the high concentration at a relatively high flowrate, APP Holding Tank 1 emissions were the greatest by nearly an order of magnitude (0.4 lb/hr). APP Mixing Tank 1, on the other hand, had a quite low flowrate, but with the highest THC

TABLE 8. SUMMARY OF THERMAL OXIDIZER INLET/OUTLET THC DATA

Test data	Inlet to thermal oxidizer				Outlet from thermal oxidizer			
Location								
Run No.	1	2	3	Average	1	2	3	Average
Date	9/22/97	9/23/97	9/23/97	–	9/22/97	9/23/97	9/23/97	–
Time	1450-1926	1015-1440	1710-2140	–	1450-1926	1015-1440	1710-2140	–
Stack Gas Data^a								
Moisture content, %	2.8	3.5	3.3	3.2	4.6	4.9	4.7	4.7
Volumetric flow rate, dscfm ^b	7,867	7,427	7,387	7,560	7,535	7,336	7,329	7,400
THC Concentrations (as propane)								
Maximum, ppm wet	100.0	91.7	92.9	94.9	10.0 ^c	1.1	1.4	4.2
Minimum, ppm wet	60.0	60.9	71.5	64.1	5.0 ^c	0.0	0.0	1.7
Average, ppm wet	73.0	72.3	81.5	75.6	6.3 ^c	0.1	0.2	2.2
Average, ppm dry	75.1	74.9	84.3	78.1	6.6 ^c	0.1	0.2	2.3
(as methane)								
Average, ppm dry	225.3	224.8	252.8	234.3	19.8 ^c	0.3	0.6	6.9
Emissions Data								
Average THC emission rate, lb/hr carbon equivalent	3.31	3.12	3.49	3.31	0.279 ^c	0.00432	0.00862	0.0958
Average THC emission rate (kg/hr carbon equivalent)	1.51	1.42	1.59	1.50	0.127 ^c	0.00197	0.00392	0.0435
Control efficiency, %	NA	NA	NA	NA	91.58 ^c	99.86	99.75	97.11

^aStack gas data gathered by ERG.^bAverage of PM and D/F trains.^cData taken from manual readings of instrument at extreme low end (zero point) of scale. Accuracy is questionable.

NA = Not applicable.

TABLE 9. SUMMARY OF SBS AND APP MIXING AND HOLDING TANK THC DATA

Test data	SBS Mixing Tank 11	SBS Holding Tank 3	APP Mixing Tank 1	APP Holding Tank 1
Location				
Run No.	1	1	1	2
Date	9/25/97	9/26/97	9/25/97	9/26/97
Time	1800-1859	1115-1214	1420-1520	1634-1641
Stack Gas Data				
Oxygen, %	20.9	20.9	20.9	20.9
Carbon dioxide, %	0.0	0.0	0.0	0.0
Moisture content, %	2.8	3.1	3.4	3.3
Gas stream velocity, fps	2.8	1.0	0.45	6.6
Volumetric flow rate, dscfm	40.9	29.3	7.05	89.9
THC Concentrations (as propane)				
Maximum, ppm wet	227	319	2,177	874
Minimum, ppm wet	126	168	1,253	473
Average, ppm wet	146	217	1,687	766
Average, ppm dry	150	224	1,746	792
(as methane)				
Average, ppm dry	451	672	5,239	2,376
Emissions Data				
Average THC emission rate (lb/hr carbon equivalent)	0.0344	0.0368	0.0690	0.399
Average THC emission rate (kg/hr carbon equivalent)	0.0157	0.0167	0.0314	0.181

TABLE 10. SUMMARY OF SBS AND APP COATER ROOF STACK THC DATA

Test data								
Location	SBS Coater Roof Stack				APP Coater Roof Stack			
Run No.	1	2	3	Average	1	2	3	Average
Date	9/24/97	9/25/97	9/25/97	—	9/24/97	9/24/97	9/24/97	—
Time	1443-1538	0922-1026	1040-1144	—	1335-1430	1510-1615	1631-1735	—
Stack Gas Data^a								
Moisture content, %	2.9	2.0	2.0	2.3	3.3	3.4	2.9	3.2
Volumetric flow rate, dscfm	10,816	11,614	11,401	11,277	10,879	11,070	11,197	11,049
THC Concentrations (as propane)								
Maximum, ppm wet	27.1	6.1	5.4	12.9	14.8	25.5	10.3	16.9
Minimum, ppm wet	10.9	4.1	3.9	6.3	10.4	2.4	4.0	5.6
Average, ppm wet	17.8	4.5	4.5	8.9	11.7	12.3	8.3	10.8
Average, ppm dry	18.3	4.6	4.6	9.1	12.1	12.7	8.5	11.1
(as methane)								
Average, ppm dry	55.0	13.8	13.8	27.4	36.3	38.2	25.6	33.4
Emissions Data								
Average THC emission rate (lb/hr carbon equivalent)	1.11	0.299	0.293	0.578	0.738	0.790	0.537	0.689
Average THC emission rate (kg/hr carbon equivalent)	0.505	0.136	0.133	0.263	0.335	0.359	0.244	0.313

^a Stack gas data gathered by ERG

concentrations still produced the second-highest emission rate (0.069 lb/hr). The SBS mixing and holding tanks showed the lowest emissions at 0.034 and 0.037 lb/hr, respectively.

As shown in Table 10, the SBS and APP coater roof stacks tested both had average THC concentrations near 10 ppm. Both processes experienced some spikes of up to about 25 ppm and also saw minimum concentrations fall below 5 ppm. Emission rates for the APP Coater Roof Stack ranged from 0.54 to 0.79 lb/hr. For the SBS Coater Roof Stack, emissions ranged from 0.29 to 1.1 lb/hr. Run 1 emissions were three to four times greater than those observed in Runs 2 and 3, which showed essentially similar trends.

4.0 TEST PROCEDURES

The procedures used for this field test are described in EPA Method 320 for using FTIR spectroscopy to measure HAP, the EPA Protocol for extractive FTIR testing at industrial point sources and EPA Method 25A for total gaseous organics. The objectives of the field test were to use the FTIR method to measure emissions from the processes, screen for HAP using the EPA FTIR reference spectrum library, and analyze the spectra for compounds not in the EPA library. Concentrations were reported for compounds that could be measured with FTIR reference spectra. Additionally, manual measurements of gas temperature, gas velocities, moisture, CO₂, and O₂ by ERG and MRI were used to calculate the mass emissions rates.

Midwest Research Institute used the extractive sampling system shown in Figure 4 to transport sample gas from the test ports to the FTIR instrument and the THC analyzer.

4.1 SAMPLING SYSTEM DESCRIPTION

4.1.1 Sample System Components

The sampling system consists of three separate components:

1. Two sample probe assemblies;
2. Two sample lines and pumps; and
3. A gas distribution manifold cart.

All wetted surfaces of the system are made of unreactive materials, Teflon®, stainless steel, or glass and are maintained at temperatures at or above 300° F to prevent condensation.

The sample probe assembly consists of the sample probe, a prefilter, a primary particulate filter, and an electronically actuated spike valve. The sample probe is a standard heated probe assembly with a pitot tube and thermocouple. The prefilter is a threaded piece of tubing loaded with glass wool attached to the end of sample probe. The primary filter is a Balston particulate filter with a 99 percent removal efficiency at 0.1 μm. The actuated spike valve is controlled by a radio transmitter connected to a switch on the sample manifold cart. All sample probe assembly components are attached to or enclosed in an insulated metal box.

The sample lines are standard heated sample lines with three 3/8-in. Teflon tubes in 10, 25, 50, and 100 foot (ft) lengths. The pumps are heated, single-headed diaphragm pumps manufactured by either KNF Neuberger or Air Dimensions. These pumps can sample at rates up

to 20 liters per minute (Lpm) depending on the pressure drop created by the components installed upstream.

The gas distribution manifold was specially constructed for FTIR sampling by MRI. It is built onto a cart that can be operated inside the MRI mobile lab or in an alternate location, if necessary. The manifold consists of a secondary particulate filter, control valves, rotameters, back pressure regulators and gauges, and a mass flow controller. The manifold can control two sample gas stream inputs, eight calibration gases, and has three individual outputs for analyzers. Also on the cart are a computer work station and controls for the spike valves and mass flow controller.

4.1.2 Sample Gas Stream Flow

Exhaust gas was withdrawn through the sample probe and transported to the gas distribution manifold. Inside the manifold the gas passed through separate secondary particulate filters. Downstream of the secondary filters, part of each sample gas stream was directed to separate THC analyzers; one to measure the inlet concentration and another to measure the outlet concentration. Part of the remaining sample gas from each stream was either sent to the FTIR instrument for analysis or exhausted with the remaining portion of the gas stream being sampled (i.e., when the inlet sample was analyzed the stack sample was exhausted and vice versa). This was accomplished by rotating the gas selection valves to allow the appropriate sample gas to pass the instrument inlet port. The gas flow to the instruments was regulated by needle valves on rotameters at the manifold outlets.

4.2 SAMPLING PROCEDURES

Sampling was conducted at all sampling locations using either one of two identical, but separate, sample systems which were both connected to the main manifold (Figure 4). A single FTIR instrument and one THC analyzer were used to sample all locations. The 4-way valves on the outlets of the common manifold could be used to select sample from either location at any given time. For several of the tests, sampling was performed using both sample lines, with the FTIR and THC alternating between locations every 30 minutes. Sample flow to each instrument was controlled by the use of the rotameter needle valves.

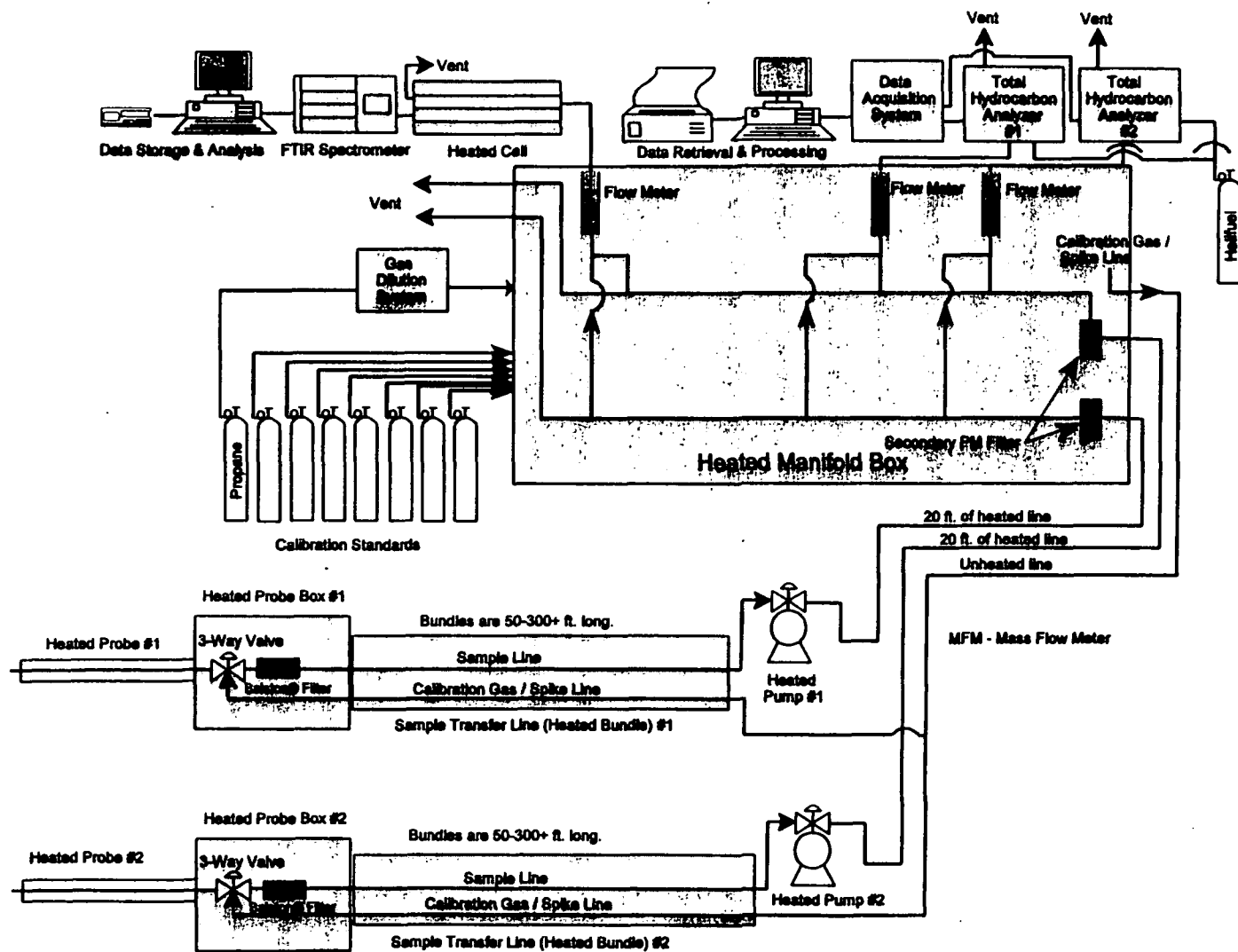


Figure 4. Extractive sampling system.

FTIR SAMPLES

Sampling was conducted using either batch or the continuous sampling procedures, described below. All data were collected according to the Method 320 sampling procedure, which is described below.

4.2.1 Batch Samples

In this procedure, the 4-way valve on the manifold outlet was turned to divert a portion of the sample flow to the FTIR cell. A positive flow to the main manifold outlet vent was maintained as the cell was filled to just above ambient pressure. The cell inlet valve was then closed to isolate the sample, the cell outlet valve was open to vent the cell to ambient pressure, the spectrum of the static sample was recorded, and then the cell was evacuated for the next sample. This procedure was repeated to collect as many samples as possible during the test run.

Batch sampling has the advantage that every sample is unique from the other samples. The time resolution of the measurements is limited by the interval required to pressurize the cell, and record the spectrum. All of the spiked samples and all of the samples for Run 2 APP Holding Tank 1 were collected using this procedure.

4.2.2 Continuous Sampling

The cell was filled as in the batch sampling procedure, but the cell inlet and outlet valves were kept open to keep gas continuously flowing through the cell. The inlet and outlet flows were regulated to keep the sample at ambient pressure. The flow through the cell was maintained at about 5 Lpm. The cell volume was about 7 L.

The FTIR instrument was automated to record spectra of the flowing sample about every 2 min. The automated analytical program was revised after the test was completed and all of the spectra were reanalyzed to measure the pollutants of interest.

This procedure with automated data collection was used for all of the unspiked testing. Because spectra were collected continuously as the sample flowed through the cell, there was mixing between consecutive samples. The interval between independent measurements (and the time resolution) depends on the sample flow rate (through the cell), and the cell volume. The following explanation is taken from Draft Performance Specification 15, which is for FTIR CEMS.

The Time Constant, TC, is the period for one cell volume to flow through the cell. The TC determines the minimum interval for complete removal of an analyte from the cell volume. It depends on the sampling rate (R_s in LPM), the cell volume (V_{cell} in L) and the analyte's chemical and physical properties.

$$TC = \frac{V_{\text{cell}}}{R_s} \quad (1)$$

Performance Specification 15 defines $5 * TC$ as the minimum interval between independent samples.

A stainless steel tube ran from the cell inlet connection point to the front of the cell. The outlet vent was at the back of the cell so that the flowing sample passed through the greatest portion of the cell volume.

4.3 ANALYTE SPIKING

Since there was little information available about HAP emissions from this source, there was no plan for validating specific HAPs at this test. MRI conducted spiking for QA purposes with using a cylinder standard of 104 ppm *p*-xylene and 4 ppm SF_6 in nitrogen.

4.3.1 Analyte Spiking Procedures

The infrared spectrum is ideally suited for analyzing and evaluating spiked samples because many compounds have very distinct infrared spectra.

The reason for analyte spiking is to provide a quality assurance check that the sampling system can transport the spiked analyte(s) to the instrument and that the quantitative analysis program can measure the analyte in the sample gas matrix. If at least 12 (independent) spiked and 12 (independent) unspiked samples are measured, then this procedure can be used to perform a Method 301 validation.³

The spike procedure follows Sections 9.2 and 13 of EPA draft Method 320. In this procedure a gas standard is measured directly in the cell. This direct measurement is then compared to measurements of the analyte in spiked samples. Ideally, the spike will comprise about 1/10 or less of the spiked sample. The expected concentration of the spiked component is determined using a tracer gas, SF_6 . The SF_6 concentration in the direct sample divided by the SF_6 concentration in the spiked sample(s) is used as the spike dilution factor (DF). The analyte

standard concentration divided by DF gives the expected value of the spiked analyte concentration.

For all testing activities on September 22, 1997, MRI generated spike gas by blending two gas streams through two separate mass flow controllers. One gas stream contained toluene and one contained SF₆. Because of this two controller approach, these spikes are likely less reliable than those performed on subsequent days. [Final spectral analysis will prove/disprove this.]

For testing on September 23 through September 26, MRI performed spiking by flowing a gas blend of SF₆ and *p*-xylene through a single mass flow controller. Because of the relatively low concentration available and low absorbance of *p*-xylene, spike flows were set to 1 to 2 Lpm, or approximately 1/6 to 1/3 of the total sample flow. The spike recovery results are presented in Table 6 in Section 3.

4.3.2 Analysis of Spiked Results

The statistical procedures in Section 6.3 of EPA Method 301 were followed to analyze the spiked and unspiked results. The application of these procedures to FTIR test data is described in Section 13 of EPA Method 320. This involved evaluating the measurement precision, determining any systematic bias in the results, and calculating a correction factor that can be applied to the results when the validated method is used.

4.3.3 Determination of Percent Recovery

The expected concentration of the spiked component was determined using the tracer gas, SF₆. In the following discussion the “direct” measurement refers to the measured concentration in a spectrum of a sample taken directly from the spike cylinder mixture.

The dilution factor, DF, was determined by the ratio of the measured SF₆ concentration in the direct measurement of the spike mixture, SF_{6(direct)}, to the measured SF₆ concentration in the spiked samples, SF_{6(spike)}.

$$DF = \frac{SF_{6(direct)}}{SF_{6(spike)}} \quad (2)$$

The direct measurement of the analyte concentration in the spike mixture divided by DF gives the expected concentration for a 100 percent recovery of the analyte spike, C_{exp}.

$$C_{\text{exp}} = \frac{\text{Analyte}_{(\text{direct})}}{\text{DF}} \quad (3)$$

where:

Analyte_(direct) = The concentration of p-xylene in from the cylinder standard.

The actual spike recoveries in Table 6 represent the percent differences between the measured analyte concentrations in the spiked samples and C_{exp}.

$$\% \text{ Recovery} = \frac{C_{\text{exp}} - \text{Calc}}{C_{\text{exp}}} \times 100 \quad (4)$$

where "Calc" is equal to the differences between the measured analyte concentrations in spiked and unspiked samples.

4.4 ANALYTICAL PROCEDURES

Analytical procedures in the EPA FTIR Protocol² were followed for this test, and programs were prepared prior to the field test for use in analyzing the data on site. The programs employ automated routines to analyze the spectra using mathematical techniques based on a K-matrix analysis to determine analyte concentrations and an estimated uncertainty for each measurement.⁵⁻⁷ After the field test the input data (reference spectra) were modified based on the real appearance of the sample spectra. The subtracted residual baseline spectra were analyzed to estimate uncertainties in the reported concentrations.

Calculated concentrations in sample spectra were corrected for differences in absorption path length and temperature between the reference and sample spectra by

$$C_{\text{corr}} = \left(\frac{L_r}{L_s} \right) \left(\frac{T_s}{T_r} \right) C_{\text{calc}}$$

where:

C_{corr} = concentration, corrected for path length and temperature

C_{calc} = concentration, initial calculation (output of the analytical program designed for the compound)

L_r = conference spectrum path length

L_s = sample spectrum path length

T_s = absolute temperature of the sample gas, K

T_r = absolute gas temperature of reference spectrum sample, K

4.4.1 Program Input

Several versions of program input data were used in analyzing the Port Arthur spectra. Some of the spectra were qualitative and so concentrations of these compounds are not presented in the results tables. Table 11 summarizes the quantitative version of program input reference data. This information was used to calculate the reported concentration results. A second qualitative version of the program input was used to gain insight into other compounds in the emissions. Results from the second version were used to compile the information summarized in Table 5.

Table 12 summarizes the input data used to evaluate the ethylene CTS spectra. This CTS analysis was used as an independent determination of the cell path length. To analyze the CTS spectra, MRI used 0.25 cm^{-1} spectra "cts0814b" and "cts0814c." These reference CTS spectra were recorded on the same dates as the toluene reference spectra used in the analysis. These spectra were deresolved to 1.0 cm^{-1} in the same way as the toluene reference spectra using Section K.2.2 of the EPA FTIR protocol. The program analyzed the main two ethylene bands centered near $2,989$ and 949 cm^{-1} . Table 12 summarizes the results of the CTS analysis. The cell path length from this analysis was used as L_s in equation 5.

4.4.2 EPA Reference Spectra

The quantitative reference spectra used in the analysis were taken from the EPA reference spectrum library (<http://134.67.104.12/html/emtic/ftir2.htm>). The original sample and background interferograms were truncated to the first 16,384 data points. The new interferograms were then Fourier transformed using Norton-Beer medium apodization and no zero filling. The transformation parameters agreed with those used to collect the sample spectra. The deresolved 1.0 cm^{-1} single beam spectra were combined with their deresolved single beam background spectra and converted to absorbance. This same procedure was used to prepare spectral standards for the HAP's and other compounds included in the preliminary analysis.

For qualitative analysis some spectra from the Hanst spectral library (Infrared Analysis, Inc.) were used.

TABLE 11. VERSION 1 OF THE PROGRAM INPUT DATA

Compound name	File name	Region No.	ISC * = arbitrary	Reference	
				Meters	T (K)
Water	194csub	1,2,3	100*		
Carbon monoxide	co20829a	1	167.1	22	394
Sulfur dioxide	198c1bsi	2	90.3	22	394
Carbon dioxide	194b4a_b	1,2,3	850	11.2	373
Formaldehyde	087b4anb	3	100	11.25	373
Benzene	015a4ara	3	496.6	3	298
Methane	196c1bsd	3	16.09	22	394
Carbonyl sulfide	030a4ase	1	19.5	3	298
Toluene	153a4arc	3	103.0	3	298
Methyl chloride	107a4asa	3	501.4	3	298
Methyl chloroform	108a4asc	2	98.8	3	298
1,1-dichloroethane	086b4asa	2	499.1	2.25	373
1,3-butadiene	023a4asc	2	98.4	3	298
Methanol	104a4ase	2	20.1	3	298
Propane ^a	prophan	3	39.3	3	298
Cumene	046a4asc	3	96.3	3	298
Ethyl benzene	077a4arb	3	515.5	3	298
Hexane	095a4asd	3	101.6	3	298
Methylene chloride	117a4asa	2	498.5	3	298
Propionaldehyde	140b4anc	3	99.4	2.25	373
Styrene	147a4asb	2	550.7	3	298
1,1,2,2-tetrachloroethane	150b4asb	2	493.0	2.25	373
p-Xylene	173a4asa	2	488.2	3	298
o-Xylene	171a4asa	3	497.5	3	298
m-Xylene	172a4arh	2	497.8	3	298
Isooctane	165a4asc	3	101.4	3	298
Ethylene	C0926c	2	20.1	7.46	388
SF ₆	Sf6_002	2	1.0029	22	394
Ammonia	174c1asc	2	10.0	20	388

^aFrom Infrared Analysis library.

TABLE 11. (continued)

Region No.	Upper cm-1	Lower cm-1
1	2142.0	2035.6
2	1275.0	789.3
3	3160.8	2650.1

TABLE 12. PROGRAM INPUT FOR ANALYSIS OF CTS SPECTRA AND PATH LENGTH DETERMINATION

Compound name	File name	ASC	ISC	% Difference
Ethylene ^a	cts0814b.spc	1.007	1.014	0.7349
Ethylene	cts0814c.spc	1.007	0.999	0.7350

^aThis spectrum was used in the analysis of the Port Arthur CTS spectra

4.5 FTIR SYSTEM

The FTIR system used in this field test was a KVB/Analect RFX-40 interferometer. The gas cell is a heated variable path (D-22H) gas cell from Infrared Analysis, Inc. The path length of 36 laser passes was used for measurement at both locations. The inside of the cell walls have been treated with a Teflon[®] coating to minimize potential analyte losses. A mercury/cadmium/telluride (MCT) liquid nitrogen detector was used. Spectra was collected at 1.0 cm⁻¹, the highest resolution of the RFX-40 system. The cell was maintained at 240°F throughout the test series.

The optical path length was measured by shining a He/Ne laser into the cell and adjusting the mirror tilt until the desired number of passes was obtained. The path length in meters was then calculated by comparing calibration transfer standard (CTS, ethylene in nitrogen) spectra measured in the field to CTS spectra in the EPA reference spectrum library. Section 5.2 (QA/QC procedures) shows results of these calculations.

4.6 CONTINUOUS EMISSIONS MONITORING FOR TOTAL HYDROCARBONS (THC)

The THC sampling was conducted continuously by taking a split of the gas used for the FTIR sampling. Sample gas was directed to the THC analyzer through a separate set of rotameters and control valves. A summary of the specific procedures used is given below.

4.6.1 Components

A brief description of each system component follows.

1. **THC Analyzer**—The THC concentration is measured using a flame ionization detector (FID). MRI used two J.U.M. Model VE-7 instruments. The THC analyzers were operated on the zero to 100 ppm and 1,000 ppm ranges throughout the test period. The fuel for the FID is 40 percent hydrogen and 60 percent helium mixture.

2. **Data Acquisition System**—MRI uses LABTECH notebook (Windows version), which is an integrated system that provides data acquisition, monitoring and control. The system normally writes data to a disk in the background while performing foreground tasks or displaying data in real time. This system runs on a Pentium computer with a 700- megabyte hard drive and expanded memory.

3. **Calibration Gases**—Calibration gases were prepared from an EPA Protocol 1 cylinder of propane using an Environics Model 2020 gas dilution system which complies with the requirements of EPA Method 205. High, Medium and Low standards gases were generated to perform analyzer calibration checks.

The calibration gases were generated from 5,278 ppm propane in nitrogen standard. The raw data are reported in ppm as propane.

5.0 SUMMARY OF QA/QC PROCEDURES

5.1 SAMPLING AND TEST CONDITIONS

Before the test, sample lines were checked for leaks and cleaned by purging with moist air (250°F). Following this, the lines were checked for contamination using dry nitrogen. This is done by heating the sampling lines to 250°F and purging with dry nitrogen. The FTIR cell was filled with some of the purging nitrogen and the spectrum of this sample was collected. This single beam spectrum was converted to absorbance using a spectral background of pure nitrogen (99.9 percent) taken directly from a cylinder. The lines were checked again on site before sampling, after each change of location, and after spiking.

During sampling, spectra of at least 10 different samples were collected during each hour, except for Run 2 on the APP Holding Tank 1, for which batch collection was necessary.

Each spectrum was assigned a unique file name and written to the hard disk and a backup disk under that file name. Each interferogram was also saved under a file name that identifies it with its corresponding absorbance spectrum. All background spectra and calibration spectra were also stored on disks with their corresponding interferograms.

Notes on each calibration and sample spectrum were recorded on hard copy data sheets. Below are listed some sampling and instrument parameters that were documented in these records.

Sampling Conditions

- Line temperature
- Process conditions
- Sample flow rate
- Ambient pressure
- Time of sample collection

Instrument Configuration

- Cell volume (for continuous measurements)
- Cell temperature
- Cell path length
- Instrument resolution
- Number of scans co-added

- Length of time to measure spectrum
- Time spectrum was collected
- Time and conditions of recorded background spectrum
- Time and conditions of relevant CTS spectra
- Apodization

Hard copy records were also kept of all flue gas measurements, such as sample flow, temperature, moisture and diluent data.

Effluent was allowed to flow through the entire sampling system for at least 5 min before a sampling run started or after changing to a different test location. FTIR spectra were monitored in an effort to limit deviations in the spectral baseline to no greater than ± 5 percent ($-0.02 < \text{absorbance} < +0.02$). When these limits were exceeded, sampling was interrupted and a new background spectrum was collected. The run was then resumed until completed or until it was necessary to collect another background spectrum.

5.2 FTIR SPECTRA

For a detailed description of QA/QC procedures relating to data collection and analysis, refer to the "Protocol For Applying FTIR Spectrometry in Emission Testing."²

A spectrum of the calibration transfer standard (CTS) was recorded at the beginning and end of each test day. The CTS gas was 104.4 ppm ethylene in nitrogen. The CTS spectrum provided a check on the operating conditions of the FTIR instrumentation, e.g., spectral resolution and cell path length. Ambient pressures were recorded whenever a CTS spectrum was collected. The CTS spectra were compared to each other and to CTS spectra in the EPA library. These comparisons are used to quantify differences between the library spectra and the field spectra, and to track any day to day changes in the optical system as they occur.

Using known input parameters for ethylene concentration (104.4 ppm) and cell temperature (240°F, or 388K), analysis over the spectral regions of 842.5 to 1,107.3 and 2,984.4 to 2,992.4 wavenumbers was performed. An average pathlength of 7.53 m was determined, with no individual CTS spectrum varying from the average by more than 5 percent, thus meeting the Method 320 stability criteria. Table 13 shows the daily CTS results.

Two copies of all interferograms, processed backgrounds, sample spectra, and the CTS were stored on separate computer disks. Additional copies of sample and CTS absorbance spectra

TABLE 13. RESULTS OF THE CTS PATH LENGTH DETERMINATION

CTS spectra 104.4 ppm Ethylene	Path length calculations		
	Meters	Delta ^a	% Delta
C0922A	7.47	-0.07	-0.87
C0923A	7.66	0.13	1.68
C0923B	7.82	0.28	3.76
C0923C ^b	6.87	-0.66	-8.76
C0923D ^b	6.86	-0.67	-8.90
C0923E	7.33	-0.21	-2.75
C0923F	7.31	-0.22	-2.92
C0924A	7.59	0.05	0.73
C0924B	7.63	0.10	1.27
C0924C	7.35	-0.18	-2.44
C0924D	7.33	-0.21	-2.78
C0925A	7.58	0.05	0.67
C0925B	7.76	0.23	3.01
C0925C	7.36	-0.18	-2.34
C0925D	7.31	-0.23	-3.00
C0926A	7.81	0.27	3.63
C0926B	7.80	0.26	3.52
C0926C	7.49	-0.05	-0.63
C0926D	7.49	-0.04	-0.54
Average path length (M)	7.53		
Standard deviation	0.188		

^aThe difference between the calculated and average values.

^bSpectra C0923C and C0923D were not included in the average because they deviated by more than 5 percent from the average. Spectra A, B, E, and F meet the Method 320 requirement for September 23, 1997.

were also stored for data analysis. Sample absorbance spectra can be regenerated from the raw interferograms, if necessary.

To measure HAPs detected in the gas stream, MRI used spectra from the EPA library, when available.

5.3 METHOD 25A

5.3.1 Initial Checks

Before starting the first run, the following system checks were performed.

1. Zero and Span check of the analyzer;
2. Analyzer linearity check at intermediate levels;
3. Response time of the system; and
4. Calibration criterion for Method 25A is ± 5 percent of calibration gas value.

5.3.2 Daily Checks

The following checks were made for each test run.

1. Zero/Span calibration and Linearity check prior to each test run; and
2. Final Zero and Span calibrations of the analyzer at the end of each test run.

The difference between initial and final zero and span checks agreed within ± 3 percent of the instrument span.

6.0 REFERENCES

1. Test Method 320 (Draft) "Measurement of Vapor Phase Organic and Inorganic Emissions by Extractive Fourier Transform Infrared (FTIR) Spectroscopy," EPA Contract No. 68-D2-0165, Work Assignment 3-08, September, 1996.
2. "Protocol For The Use of FTIR Spectrometry to Perform Extractive Emissions Testing at Industrial Sources," Revised, EPA Contract No. 68-D2-0165, Work Assignment 3-12, September, 1996.
3. "Computer-Assisted Quantitative Infrared Spectroscopy," Gregory L. McClure (ed.), ASTM Special Publication 934 (ASTM), 1987.
4. "Multivariate Least-Squares Methods Applied to the Quantitative Spectral Analysis of Multicomponent Mixtures," Applied Spectroscopy, 39(10), 73-84, 1985.
5. "An Examination of a Least Squares Fit FTIR Spectral Analysis Method," G. M. Plummer and W. K. Reagen, *Air and Waste Management Association*, Paper Number 96-WA65.03, 1996.
6. "Method 25A—Determination of Total Gaseous Organic Concentration Using a Flame Ionization Analyzer," 40 CFR 60, Appendix A.

APPENDIX A

FIELD DATA SHEETS FOR STACK FLOW MEASUREMENTS

40 CFR 60, APPENDIX A, METHOD 2* - GAS STREAM VELOCITY AND VOLUMETRIC FLOW RATE

MRI Project No. 3804.21.04.03
Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
Sampling Location: APP Line - Modified Bitumen Mixing Tank M1 Outlet Vent E2B (E6)

Run No. 1
Date: 09/25/97

Type S Pitot Tube No.	8-2-96-5	Temperature Meter No.	Y-3917	Barometer No.	X-4029
Pitot Tube Coefficient (Cp):	0.84	Elevation Change** from Barometer Location to Sampling Location:	20 feet		
Thermocouple No.	8-2-96-5T	Cross Sectional Area of the Duct at Sampling Location:	0.328 ft²		
Carbon Dioxide Concentration By Volume, Dry Basis:	0.0 %	Gas Mol. Weight, Dry Basis (Md):	28.965 lb/lb-mole		
Oxygen Concentration By Volume, Dry Basis:	20.9 %				

FIRST TRAVERSE - START OF RUN

Start Time: 1310	Stop Time: 1350
Barometric Pressure at Barometer Location:	29.94 in. Hg
Barometric Pressure at Sampling Location:	29.92 in. Hg
Velocity Head at Centroid:	0.00 in. w.c.
Total Pressure at Centroid:	-0.10 in. w.c.
Static Pressure:	-0.100 in. w.c.
Absolute Pressure in Duct (Ps):	29.91 in. Hg
Dry Bulb Temperature:	107 °F
Wet Bulb Temperature:	86 °F
Water Vapor Concentration By Volume:	3.42 %
Gas Mol. Weight, Wet Basis (Ms):	28.590 lb/lb-mole

[illegible]

Average Rotation Angle:	NR
Average Velocity:	26.8 ft/min
Volumetric Flow Rate:	8.76 acfm
Volumetric Flow Rate:	7.28 scfm
Volumetric Flow Rate:	7.03 dscfm
Volumetric Flow Rate:	0.199 dry std. m ³ /min.

SECOND TRAVERSE - END OF RUN

Start Time: 1620	Stop Time: 1640
Barometric Pressure at Barometer Location:	29.93 in. Hg
Barometric Pressure at Sampling Location:	29.91 in. Hg
Velocity Head at Centroid:	0.00 in. w.c.
Total Pressure at Centroid:	-0.10 in. w.c.
Static Pressure:	-0.100 in. w.c.
Absolute Pressure in Duct (Ps):	29.90 in. Hg
Dry Bulb Temperature:	104 °F
Wet Bulb Temperature:	85 °F
Water Vapor Concentration By Volume:	3.36 %
Gas Mol. Weight, Wet Basis (Ms):	28.597 lb/lb-mole

[illegible]

Average Velocity:	26.9 ft/min
Volumetric Flow Rate:	8.80 acfm
Volumetric Flow Rate:	7.30 scfm
Volumetric Flow Rate:	7.06 dscfm
Volumetric Flow Rate:	0.200 dry std. m ³ /min.

RESULTS FOR RUN

Average Volumetric Flow Rate: 422.8 dry std. ft³/hr.
Average Volumetric Flow Rate: 11.97 dry std. m³/hr.

Deviation of the flow rate after the run from the one before the run: 0.5 %

COMMENTS: No readings (NR) were obtained with a Type S pitot tube because of the very low flow rate. Absence of cyclonic flow could not be determined, and a hot wire anemometer was used to measure velocity and total pressure (with pitot tube).

- 40 CFR 60, Appendix A, Method 3 is used for the determination of dry molecular weight, and ASTM Method E337-84(1996) is used for determination of moisture content.

Positive values for locations above the barometer and negative values for locations below the barometer are entered here. (Computations reverse the signs to yield correct results.)

40 CFR 60, APPENDIX A, METHOD 2* - GAS STREAM VELOCITY AND VOLUMETRIC FLOW RATE

MRI Project No. 3804.21.04.03
Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
Sampling Location: SBS Line - Modified Bitumen Mixing Tank M11 Outlet Vent (E5)

Run No. 1
Date: 09/25/97

Type S Pitot Tube No.	8-2-98-5	Temperature Meter No.	Y-3917	Barometer No.	X-4029
Pitot Tube Coefficient (Cp):	0.84	Elevation Change** from Barometer Location to Sampling Location:	20 feet		
Thermocouple No.	8-2-98-5T	Cross Sectional Area of the Duct at Sampling Location:	0.328 ft ²		
Carbon Dioxide Concentration By Volume, Dry Basis:	0.0 %	Gas Mol. Weight, Dry Basis (Md):	28.965 lb/lb-mole		
Oxygen Concentration By Volume, Dry Basis:	20.9 %				

FIRST TRAVERSE - START OF RUN

Start Time:	Stop Time:
Barometric Pressure at Barometer Location:	in. Hg
Barometric Pressure at Sampling Location:	in. Hg
Velocity Head at Centroid:	in. w.c.
Total Pressure at Centroid:	in. w.c.
Static Pressure:	in. w.c.
Absolute Pressure in Duct (Pa):	in. Hg
Dry Bulb Temperature:	°F
Wet Bulb Temperature:	°F
Water Vapor Concentration by Volume:	%
Gas Mol. Weight, Wet Basis (M_s):	lb/lb-mole

[illegible]

Average Rotation Angle:	NR
Average Velocity:	ft/min
Volumetric Flow Rate:	acfm
Volumetric Flow Rate:	scfm
Volumetric Flow Rate:	dscfm
Volumetric Flow Rate:	dry std. m ³ /min.

SECOND TRAVERSE - END OF RUN

Start Time:	1930	Stop Time:	2000
Barometric Pressure at Barometer Location:	29.91 in. Hg		
Barometric Pressure at Sampling Location:	29.89 in. Hg		
Velocity Head at Centroid:	0.00 in. w.c.		
Total Pressure at Centroid:	-0.01 in. w.c.		
Static Pressure:	-0.010 in. w.c.		
Absolute Pressure in Duct (Ps):	29.89 in. Hg		
Dry Bulb Temperature:	94 °F		
Wet Bulb Temperature:	79 °F		
Water Vapor Concentration by Volume:	2.79 %		
Gas Mol. Weight, Wet Basis (Ms):	28.659 lb/lb-mole		

[illegible]

Average Velocity:	167 ft/min
Volumetric Flow Rate:	54.5 acfm
Volumetric Flow Rate:	42.1 scfm
Volumetric Flow Rate:	40.9 dscfm
Volumetric Flow Rate:	1.16 dry std. m ³ /min.

RESULTS FOR RUN

Average Volumetric Flow Rate: 2,456 dry std. ft³/hr.
Average Volumetric Flow Rate: 69.55 dry std. m³/hr.

Deviation of the flow rate after the run from the one before the run: NA

COMMENTS: No readings (NR) were obtained with a Type S pitot tube because of the very low flow rate. Absence of cyclonic flow could not be determined, and a hot wire anemometer was used to measure velocity and total pressure (with pitot tube).

Because of time constraints, measurements were not conducted prior to the FTIR and THC sampling.

- 40 CFR 60, Appendix A, Method 3 is used for the determination of dry molecular weight, and ASTM Method E337-84(1996) is used for determination of moisture content.

** Positive values for locations above the barometer and negative values for locations below the barometer are entered here. (Computations reverse the signs to yield correct results.)

40 CFR 60, APPENDIX A, METHOD 2* - GAS STREAM VELOCITY AND VOLUMETRIC FLOW RATE

MRI Project No. 3804.21.04.03
Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
Sampling Location: SBS Line - Modified Bitumen Holding Tank H3 Outlet Vent E19B (E3)

Run No. 1
Date: 09/26/97

Type S Pitot Tube No.	8-2-96-5	Temperature Meter No.	Y-3917	Barometer No.	X-4029
Pitot Tube Coefficient (Cp):	0.84	Elevation Change** from Barometer Location to Sampling Location:	24 feet		
Thermocouple No.	8-2-96-5T	Cross Sectional Area of the Duct at Sampling Location:	0.532 ft ²		
Carbon Dioxide Concentration By Volume, Dry Basis:	0.0 %	Gas Mol. Weight, Dry Basis (Md):	28.965 lb/lb-mole		
Oxygen Concentration By Volume, Dry Basis:	20.9 %				

FIRST TRAVERSE - START OF RUN

Start Time: 1030	Stop Time: 1100
Barometric Pressure at Barometer Location:	29.99 in. Hg
Barometric Pressure at Sampling Location:	29.97 in. Hg
Velocity Head at Centroid:	0.00 in. w.c.
Total Pressure at Centroid:	-0.02 in. w.c.
Static Pressure:	-0.020 in. w.c.
Absolute Pressure in Duct (Pa):	29.96 in. Hg
Dry Bulb Temperature:	93 °F
Wet Bulb Temperature:	82 °F
Water Vapor Concentration By Volume:	3.27 %
Gas Mol. Weight, Wet Basis (M _s):	28.606 lb/lb-mole

[illegible]

Average Rotation Angle:	NR
Average Velocity:	285 ft/min
Volumetric Flow Rate:	151 acfm
Volumetric Flow Rate:	135 scfm
Volumetric Flow Rate:	131 dscfm
Volumetric Flow Rate:	3.70 dry std. m ³ /min.

SECOND TRAVERSE - END OF RUN

Start Time: 1345	Stop Time: 1405
Barometric Pressure at Barometer Location:	29.98 in. Hg
Barometric Pressure at Sampling Location:	29.96 in. Hg
Velocity Head at Centroid:	0.00 in. w.c.
Total Pressure at Centroid:	-0.06 in. w.c.
Static Pressure:	-0.060 in. w.c.
Absolute Pressure in Duct (Pa):	28.95 in. Hg
Dry Bulb Temperature:	97 °F
Wet Bulb Temperature:	81 °F
Water Vapor Concentration by Volume:	2.97 %
Gas Mol. Weight, Wet Basis (M _s):	28.639 lb/lb-mole

[illegible]

Average Velocity:	62.0 ft/min
Volumetric Flow Rate:	33.0 acfm
Volumetric Flow Rate:	30.2 scfm
Volumetric Flow Rate:	29.3 dscfm
Volumetric Flow Rate:	0.830 dry std. m ³ /min.

RESULTS FOR RUN

Average Volumetric Flow Rate: 1,758 dry std. ft³/hr.
Average Volumetric Flow Rate: 49.79 dry std. m³/hr.

Deviation of the flow rate after the run from the one before the run: NA

COMMENTS: No readings (NR) were obtained with a Type S pitot tube because of the very low flow rate. Absence of cyclonic flow could not be determined, and a hot wire anemometer was used to measure velocity and total pressure (with pitot tube).

Results from the first traverse are not representative of normal operating conditions. An access door at the top of the tank in the outlet vent breech was open during the traverse. This was discovered shortly after FTIR and THC sampling started. The door was closed and FTIR and THC sampling was restarted. Because of time constraints, the first traverse was not repeated.

- 40 CFR 60, Appendix A, Method 3 is used for the determination of dry molecular weight, and ASTM Method E337-84(1996) is used for determination of moisture content.
- ** Positive values for locations above the barometer and negative values for locations below the barometer are entered here. (Computations reverse the signs to yield correct results.)

40 CFR 60, APPENDIX A, METHOD 2* -

Run No. 7

Date: 09-25-97

Date: 09-25-97

7/5-

Temperature Meter No. ~~3~~-3912

Thermocouple No. 8-2-96-55

Barometer No. X-4029

20 feet

0.328 ft³

0.0 %

20.9 %

SECOND TRAVERSE - END OF RUN

Start Time: 1620 Stop Time: 1640

P_{bar}: 29.93 in. Hg

Δp : 0.00 in. H₂O

P: -0.10 in. H₂O

Temperature: 104 °F

Temperature: 85 °F

Initial: NOLTERS Final: NO LEEKS

[illegible]

- * * Enter positive values for locations above barometer and negative values for locations below barometer.

Comments: Flow rate too low for using pitot tube. Used hot wire anemometer for velocity and total pressure.

M2TSWBDB.WPD September 18, 1997 (rev. M2TSE3.WPD September 18, 1997)

40 CFR 60, APPENDIX A, METHOD 2* -
GAS STREAM VELOCITY AND VOLUMETRIC FLOW RATE FIELD DATA SHEET

MRI Project No. 3804.21.04.03 Run No. 1
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas Date: 09-26-97
 Sampling Location: APP Line - Modified Bitumen Holding Tank H1 Outlet E1B (E4)
 Operator(s): J. Surman B. Teaford
 Type S Pitot Tube No. 8-2-96-5 Temperature Meter No. Y-3917
 Pitot Tube Coefficient (C_p): 0.84 Thermocouple No. 8-2-96-51
 Hot-wire Anemometer No. 4560 *** Barometer No. X-4029
 Elevation Change** from Barometer Location to Sampling Location: 16 feet
 Cross Sectional Area of Duct at Sampling Location: 0.349 ft²
 Carbon Dioxide Concentration By Volume, Dry Basis: 0.0 %
 Oxygen Concentration By Volume, Dry Basis: 20.9 %

FIRST TRAVERSE - START OF RUN

Start Time: 1250 Stop Time: 1315
 Barometric Pressure (P_{bar}) at Barometer Location: 29.98 in. Hg
 Velocity Head (Δp) at Centroid of Duct: 0.01 in. H₂O
 Total Pressure (P) at Centroid of Duct: -0.04 in. H₂O
 Dry Bulb Temperature: 129 °F
 Wet Bulb Temperature: 90 °F
 Leak Checks - Initial: NO LEAKS Final: NO LEAKS

Traverse Point Number	Velocity Head, (Δp), in. H ₂ O	Gas Stream Temp. (t_s), °F	Rotation Angle, α
1	320 ft/min	327	NR ↓
2	325	327	
3	410	327	
4	430	327	
5	445	327	
6	390	327	

SECOND TRAVERSE - END OF RUN

Start Time: 1828 Stop Time: 1844
 Barometric Pressure (P_{bar}) at Barometer Location: 29.97 in. Hg
 Velocity Head (Δp) at Centroid of Duct: 0.01 in. H₂O
 Total Pressure (P) at Centroid of Duct: -0.04 in. H₂O
 Dry Bulb Temperature: 125 °F
 Wet Bulb Temperature: 89 °F
 Initial: NO LEAKS Final: NO LEAKS

Traverse Point Number	Velocity Head, (Δp), in. H ₂ O	Gas Stream Temp. (t_s), °F
1	340 ft/min	316
2	363	316
3	395	316
4	420	316
5	435	316
6	400	316

* 40 CFR 60, Appendix A, Method 3 is used for the determination of dry gas molecular weight, and ASTM Method E337-84(1996) is used for the determination of moisture content.

** Enter positive values for locations above barometer and negative values for locations below barometer.

*** TSI, Inc. VelocicalPlus Model 8360, S/N 96060280

Comments: *Flow rate too low for using pitot tube. Used hot wire anemometer for velocity and total pressure.*

M2TSWBDB.WPD September 18, 1997 (rev. M2TSE3.WPD September 18, 1997)

**40 CFR 60, APPENDIX A, METHOD 1 -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Thermal Oxidizer Inlet Duct (E1)
 Date: 09/22/97
 Measured by J. Surman

Port - A

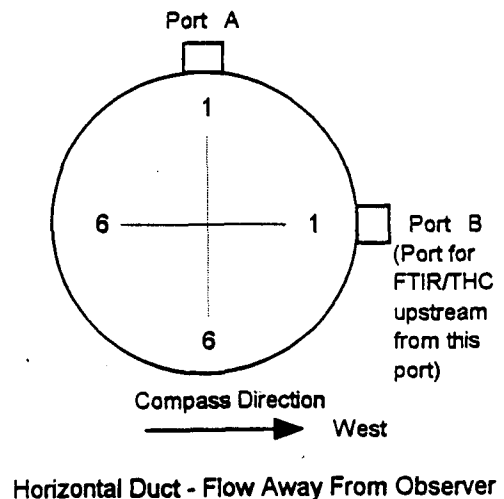
Inside of far wall to outside reference point (distance Li): 39.000 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 35.750 inches

Port - B

Inside of far wall to outside reference point (distance Li): 39.000 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 35.750 inches
 Nearest flow disturbance upstream from ports: 288 inches, (8.1 D)
 Nearest flow disturbance downstream from ports: 72 inches, (2.0 D)
 Minimum number of points for velocity (nonparticulate) traverses: 12
 Minimum number of points for particulate traverses: 12

Inside diameter of the duct: 35.75 inches
 Number of traverse points to be used on a diameter: 6
 Length of port from reference point to inside surface of duct: 3.25 inches
 Cross sectional area of sampling location: 6.971 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	4.4%	4.81
2	14.6%	8.49
3	29.6%	13.83
4	70.4%	28.42
5	85.4%	33.76
6	95.6%	37.44



Comments: Note that the sampling location for FTIR and THC is 35 inches upstream from this cross section.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Thermal Oxidizer Outlet - Stack (E2)
 Date: 09/22/97
 Measured by J. Surman

Port - South

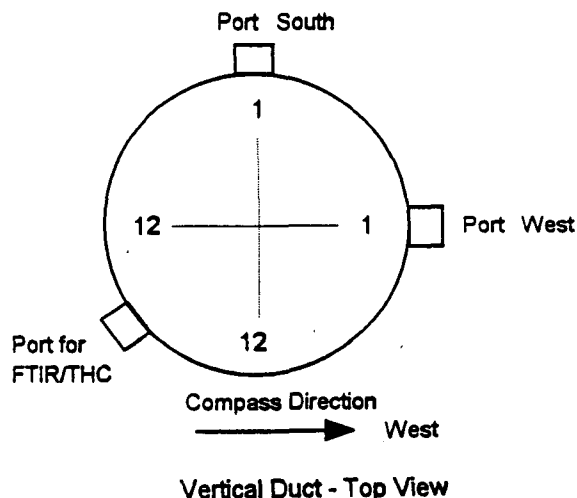
Inside of far wall to outside reference point (distance Li): 39.000 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 35.750 inches

Port - West

Inside of far wall to outside reference point (distance Li): 39.000 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 35.750 inches
 Nearest flow disturbance upstream from ports: 162 inches, (4.5 D)
 Nearest flow disturbance downstream from ports: 42 inches, (1.2 D)
 Minimum number of points for velocity (nonparticulate) traverses: 16
 Minimum number of points for particulate traverses: 24

Inside diameter of the duct: 35.75 inches
 Number of traverse points to be used on a diameter: 12
 Length of port from reference point to inside surface of duct: 3.25 inches
 Cross sectional area of sampling location: 6.971 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	2.8%	4.25
2	6.7%	5.64
3	11.8%	7.47
4	17.7%	9.59
5	25.0%	12.19
6	35.6%	15.96
7	64.4%	26.29
8	75.0%	30.06
9	82.3%	32.66
10	88.2%	34.78
11	93.3%	36.61
12	97.2%	38.00



Comments: Note that the sampling location for FTIR and THC is 76 inches below (upstream from) this cross section.

40 CFR 60, APPENDIX A, METHODS 1 and 1A - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

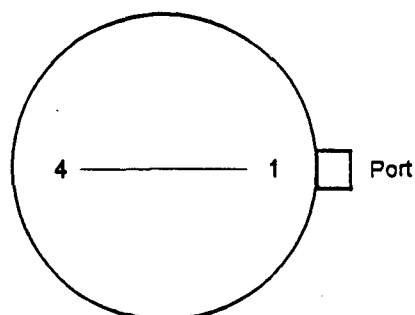
MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: SBS Line - Modified Bitumen Holding Tank H3 Outlet E19B (E3)
 Date: 09/22/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 12.625 inches
 Inside of near wall to outside reference point (distance Lo): 2.750 inches
 Duct inside diameter (Li - Lo): 9.875 inches

Nearest flow disturbance upstream from ports: 192 inches, (19.4 D)
 Nearest flow disturbance downstream from ports: 96 inches, (9.7 D)
 Minimum number of points for velocity (nonparticulate) traverses: 8
 Minimum number of points for particulate traverses: 8

Inside diameter of the duct: 9.88 inches
 Number of traverse points to be used on a diameter: 4
 Length of port from reference point to inside surface of duct: 2.75 inches
 Cross sectional area of sampling location: 0.532 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.7%	3.41
2	25.0%	5.22
3	75.0%	10.16
4	93.3%	11.96



Compass Direction
 → South

Horizontal Duct - Flow Away From Observer

Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

**40 CFR 60, APPENDIX A, METHODS 1 and 1A -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

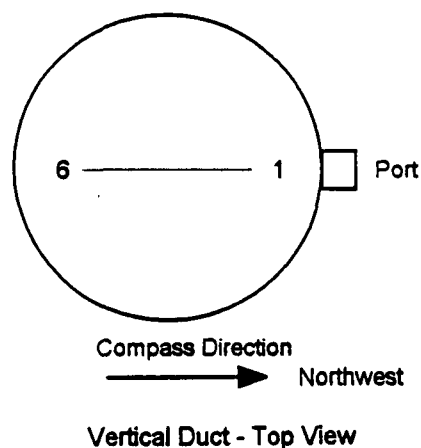
MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: APP Line - Modified Bitumen Holding Tank H1 Outlet E1B (E4)
 Date: 09/22/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 10.500 inches
 Inside of near wall to outside reference point (distance Lo): 2.500 inches
 Duct inside diameter (Li - Lo): 8.000 inches

Nearest flow disturbance upstream from ports: 52 inches, (6.5 D)
 Nearest flow disturbance downstream from ports: 20 inches, (2.5 D)
 Minimum number of points for velocity (nonparticulate) traverses: 12
 Minimum number of points for particulate traverses: 16

Inside diameter of the duct: 8.00 inches
 Number of traverse points to be used on a diameter: 6
 Length of port from reference point to inside surface of duct: 2.50 inches
 Cross sectional area of sampling location: 0.349 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.3%	3.00
2	14.6%	3.67
3	29.6%	4.87
4	70.4%	8.13
5	85.4%	9.33
6	93.8%	10.00



Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

**40 CFR 60, APPENDIX A, METHODS 1 and 1A -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

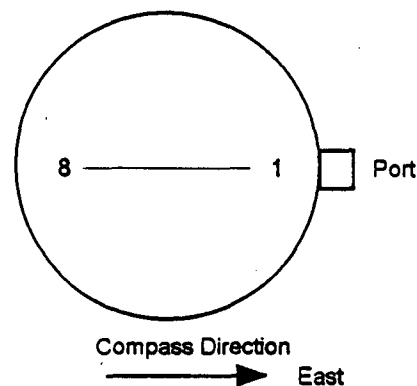
MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: SBS Line - Modified Bitumen Mixing Tank M11 Outlet (E5)
 Date: 09/22/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 10.250 inches
 Inside of near wall to outside reference point (distance Lo): 2.500 inches
 Duct inside diameter (Li - Lo): 7.750 inches

Nearest flow disturbance upstream from ports: 18 inches, (2.3 D)
 Nearest flow disturbance downstream from ports: 20 inches, (2.6 D)
 Minimum number of points for velocity (nonparticulate) traverses: 16
 Minimum number of points for particulate traverses: 24

Inside diameter of the duct: 7.75 inches
 Number of traverse points to be used on a diameter: 8
 Length of port from reference point to inside surface of duct: 2.50 inches
 Cross sectional area of sampling location: 0.328 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.5%	3.00
2	10.5%	3.31
3	19.4%	4.00
4	32.3%	5.00
5	67.7%	7.75
6	80.6%	8.75
7	89.5%	9.44
8	93.5%	9.75



Horizontal Duct - Flow Away From Observer

Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct configuration and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

**40 CFR 60, APPENDIX A, METHODS 1 and 1A -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

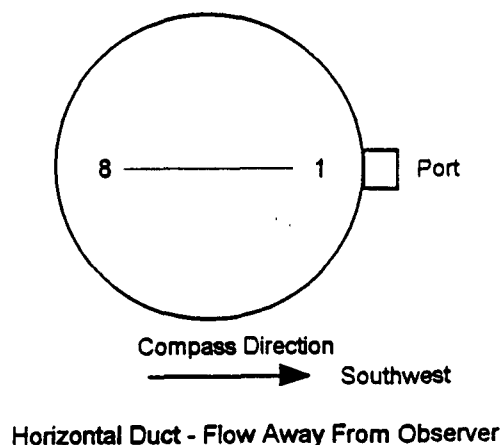
MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: APP Line - Modified Bitumen Mixing Tank M1 Outlet E2B (E6)
 Date: 09/22/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 10.500 inches
 Inside of near wall to outside reference point (distance Lo): 2.750 inches
 Duct inside diameter (Li - Lo): 7.750 inches

Nearest flow disturbance upstream from ports: 44 inches, (5.7 D)
 Nearest flow disturbance downstream from ports: 27 inches, (3.5 D)
 Minimum number of points for velocity (nonparticulate) traverses: 16
 Minimum number of points for particulate traverses: 20

Inside diameter of the duct: 7.75 inches
 Number of traverse points to be used on a diameter: 8
 Length of port from reference point to inside surface of duct: 2.75 inches
 Cross sectional area of sampling location: 0.328 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.5%	3.25
2	10.5%	3.56
3	19.4%	4.25
4	32.3%	5.25
5	67.7%	8.00
6	80.6%	9.00
7	89.5%	9.69
8	93.5%	10.00



Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Coater Vent E10S for APP Line (E7)
 Date: 09/23/97
 Measured by J. Surman

Port - East

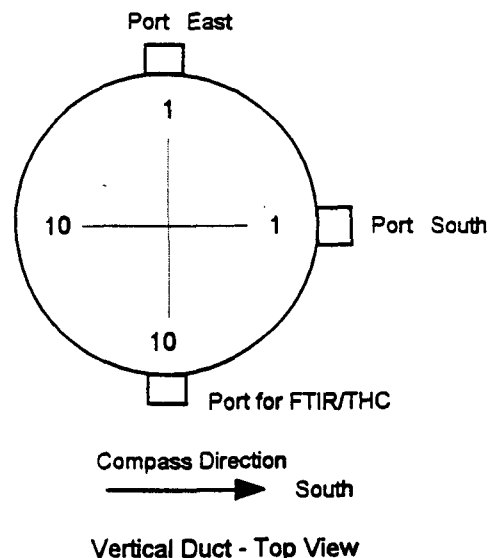
Inside of far wall to outside reference point (distance Li): 32.125 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 28.875 inches

Port - South

Inside of far wall to outside reference point (distance Li): 32.375 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 29.125 inches
 Nearest flow disturbance upstream from ports: 166 inches, (5.7 D)
 Nearest flow disturbance downstream from ports: 54 inches, (1.9 D)
 Minimum number of points for velocity (nonparticulate) traverses: 16
 Minimum number of points for particulate traverses: 20

Inside diameter of the duct: 29.00 inches
 Number of traverse points to be used on a diameter: 10
 Length of port from reference point to inside surface of duct: 3.25 inches
 Cross sectional area of sampling location: 4.587 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	3.4%	4.25
2	8.2%	5.62
3	14.6%	7.50
4	22.6%	9.81
5	34.2%	13.16
6	65.8%	22.34
7	77.4%	25.69
8	85.4%	28.00
9	91.8%	29.88
10	96.6%	31.25



Comments: Note that the sampling location for FTIR and THC is 11 inches below (upstream from) this cross section.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Coater Vent E20S for SBS Line (E8)
 Date: 09/23/97
 Measured by J. Surman

Port - East

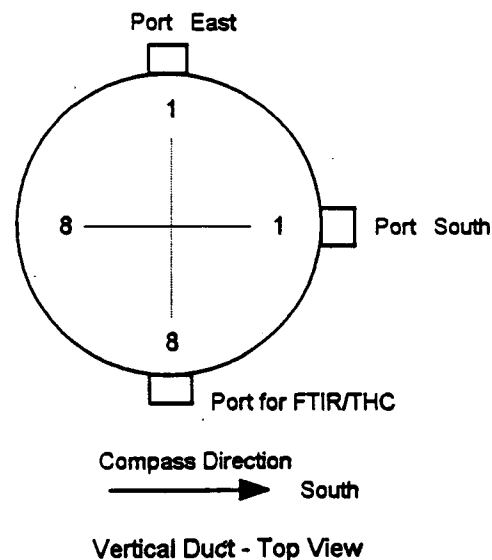
Inside of far wall to outside reference point (distance Li): 32.125 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 28.875 inches

Port - South

Inside of far wall to outside reference point (distance Li): 32.375 inches
 Inside of near wall to outside reference point (distance Lo): 3.250 inches
 Duct inside diameter (Li - Lo): 29.125 inches
 Nearest flow disturbance upstream from ports: 176 inches, (6.1 D)
 Nearest flow disturbance downstream from ports: 65 inches, (2.2 D)
 Minimum number of points for velocity (nonparticulate) traverses: 12
 Minimum number of points for particulate traverses: 16

Inside diameter of the duct: 29.00 inches
 Number of traverse points to be used on a diameter: 8
 Length of port from reference point to inside surface of duct: 3.25 inches
 Cross sectional area of sampling location: 4.587 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	3.4%	4.25
2	10.5%	6.29
3	19.4%	8.87
4	32.3%	12.62
5	67.7%	22.88
6	80.6%	26.63
7	89.5%	29.21
8	96.6%	31.25



Comments: Note that the sampling location for FTIR and THC is 14 inches below (upstream from) this cross section.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
Sampling Location: Thermal Oxidizer Inlet Duct (E1)
Date: 09/20/97
Measured by J. Surman

Port - A

Inside of far wall to outside reference point (distance Li): 42.000 inches *39.0*
Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
Duct inside diameter (Li - Lo): 36.000 inches *35.75*

Port - B

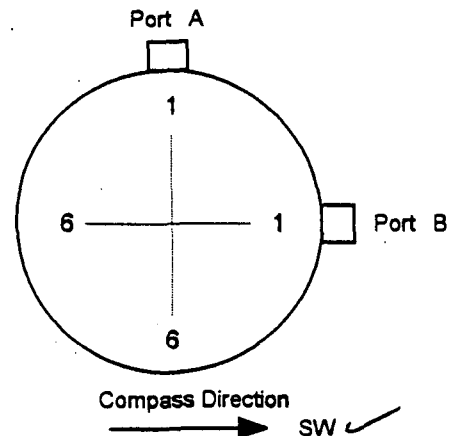
Inside of far wall to outside reference point (distance Li): 42.000 inches *39.0*
Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
Duct inside diameter (Li - Lo): 36.000 inches *35.75*
Nearest flow disturbance upstream from ports: 288 inches, (8.0 D) ✓
Nearest flow disturbance downstream from ports: 72 inches, (2.0 D) ✓
Minimum number of points for velocity (nonparticulate) traverses: 12
Minimum number of points for particulate traverses: 12

MRI - 35" 2427

Inside diameter of the duct: 36.00 inches *35.75*
Number of traverse points to be used on a diameter: 6
Length of port from reference point to inside surface of duct: 6.00 inches *3.25*
Cross sectional area of sampling location: 7.069 ft² *6.971*

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	4.4%	7.57
2	14.6%	11.27
3	29.6%	16.65
4	70.4%	31.35
5	85.4%	36.73
6	95.6%	40.43

*4.81
8.49
13.83
28.12
33.76
37.44*



Horizontal Duct - Flow Away From Observer

35"

Comments: Note that the sampling location for FTIR and THC is ~~3 feet~~ upstream from this cross section.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Thermal Oxidizer Outlet - Stack (E2)
 Date: 09/20/97
 Measured by J. Surman

Port - SW

Inside of far wall to outside reference point (distance Li): 42.000 inches 39.0
 Inside of near wall to outside reference point (distance Lo): 6.000 inches 3.25
 Duct inside diameter (Li - Lo): 36.000 inches 35.75

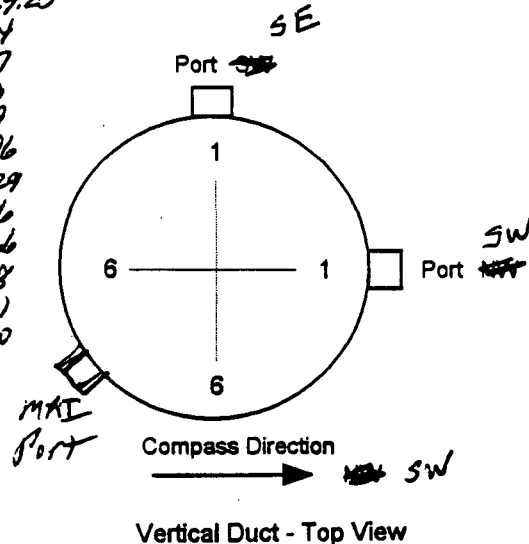
Port - NW

Inside of far wall to outside reference point (distance Li): 42.000 inches 39.0
 Inside of near wall to outside reference point (distance Lo): 6.000 inches 3.25
 Duct inside diameter (Li - Lo): 36.000 inches 35.75 MRI ERG
 Nearest flow disturbance upstream from ports: 260 inches, (452.2 D) 86 916.0
 Nearest flow disturbance downstream from ports: 80 inches, (122.2 D) 118 42
 Minimum number of points for velocity (nonparticulate) traverses: 12/6
 Minimum number of points for particulate traverses: 12/24

Inside diameter of the duct: 36.00 inches 35.75
 Number of traverse points to be used on a diameter: 6/2
 Length of port from reference point to inside surface of duct: 6.00 inches 3.25
 Cross sectional area of sampling location: 7.069 ft² 6.971

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	4.4%	7.57
2	14.6%	11.27
3	29.6%	16.65
4	70.4%	31.35
5	85.4%	36.73
6	95.6%	40.43

40.25
 56.4
 7.47
 9.59
 12.19
 15.96
 26.29
 30.26
 32.66
 34.78
 36.61
 38.00



Comments: Note that the sampling location for FTIR and THC is 12 inches below (upstream from) this cross section.

40 CFR 60, APPENDIX A, METHODS 1 and 1A - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: SBS Line - Modified Bitumen Holding Tank H3 Outlet E19B (E3)
 Date: 09/24/97
 Measured by J. Surman

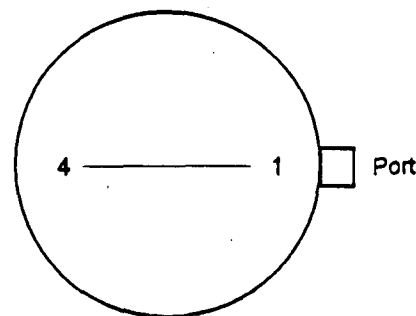
Inside of far wall to outside reference point (distance Li): 16.000 inches *12 5/8*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *2.25*
 Duct inside diameter (Li - Lo): 10.000 inches *9.875*

Nearest flow disturbance upstream from ports: 100 inches, (*19.4* D) *16 x 12 = 192*
 Nearest flow disturbance downstream from ports: 75 inches, (*7.5* D) *96*
 Minimum number of points for velocity (nonparticulate) traverses: 8 *9.7*
 Minimum number of points for particulate traverses: 8

Inside diameter of the duct: ~~10.00~~ inches *9.88*
 Number of traverse points to be used on a diameter: ~~4~~
 Length of port from reference point to inside surface of duct: ~~6.00~~ inches *2.75*
 Cross sectional area of sampling location: ~~0.545~~ ft² *0.532*

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.7%	6.67
2	25.0%	8.50
3	75.0%	13.50
4	93.3%	15.33

3.41
5.22
10.16
11.96



Compass Direction
 → *SE*

Horizontal Duct - Flow Away From Observer

Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

**40 CFR 60, APPENDIX A, METHODS 1 and 1A -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

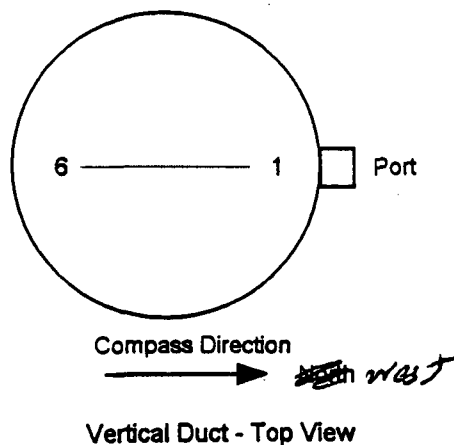
MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: APP Line - Modified Bitumen Holding Tank H1 Outlet E1B (E4)
 Date: 09/24/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 14.000 inches *10.5*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *2.5*
 Duct inside diameter (Li - Lo): 8.000 inches

 Nearest flow disturbance upstream from ports: 54 inches, (*6.5* ~~5.8~~ D) *52*
 Nearest flow disturbance downstream from ports: 16 inches, (*2.0* ~~2.0~~ D) *20*
 Minimum number of points for velocity (nonparticulate) traverses: 12 *25*
 Minimum number of points for particulate traverses: 16

 Inside diameter of the duct: 8.00 inches
 Number of traverse points to be used on a diameter: 6
 Length of port from reference point to inside surface of duct: ~~6.00~~ inches *2.50*
 Cross sectional area of sampling location: 0.349 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches	
1	6.3%	6.50	<i>3.00</i>
2	14.6%	7.17	<i>3.67</i>
3	29.6%	8.37	<i>4.87</i>
4	70.4%	11.63	<i>8.13</i>
5	85.4%	12.83	<i>9.33</i>
6	93.8%	13.50	<i>10.00</i>



Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

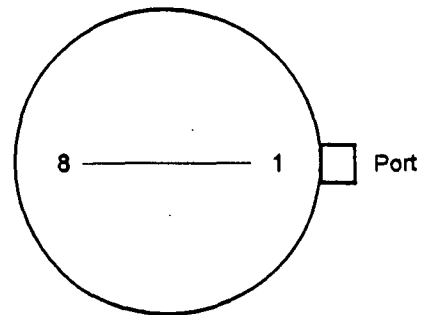
**40 CFR 60, APPENDIX A, METHODS 1 and 1A -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: SBS Line - Modified Bitumen Mixing Tank ~~M7~~ Outlet E17B (E5)
 Date: 09/24/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 14.000 inches *10.25*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *2.50*
 Duct inside diameter (Li - Lo): 8.000 inches *7.75*
 Nearest flow disturbance upstream from ports: 30 inches, (*23* ~~3.8~~ D) *18*
 Nearest flow disturbance downstream from ports: 16 inches, (*2.8* ~~2.8~~ D) *20*
 Minimum number of points for velocity (nonparticulate) traverses: 16 *2.6*
 Minimum number of points for particulate traverses: 24
 Inside diameter of the duct: ~~8.00~~ inches *7.75*
 Number of traverse points to be used on a diameter: 8
 Length of port from reference point to inside surface of duct: ~~6.00~~ inches *2.50*
 Cross sectional area of sampling location: ~~0.349~~ ft² *0.328*

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.3%	6.50
2	10.5%	6.84
3	19.4%	7.55
4	32.3%	8.59
5	67.7%	11.41
6	80.6%	12.45
7	89.5%	13.16
8	93.8%	13.50

3.00
3.31
4.00
5.00
7.75
8.75
9.44
9.75



Compass Direction
 → *NE*

Horizontal Duct - Flow Away From Observer

Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct configuration and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

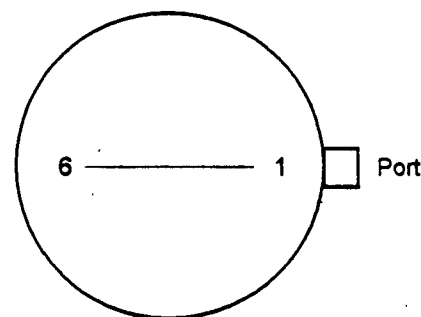
40 CFR 60, APPENDIX A, METHODS 1 and 1A - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: APP Line - Modified Bitumen Mixing Tank M1 Outlet E2B (E6)
 Date: 09/24/97
 Measured by J. Surman

Inside of far wall to outside reference point (distance Li): 14.000 inches ~~14.00~~ 10.5
 Inside of near wall to outside reference point (distance Lo): 6.000 inches 2.75
 Duct inside diameter (Li - Lo): 8.000 inches 7.75
 Nearest flow disturbance upstream from ports: 50 inches, (5.7 6.3 D) 44
 Nearest flow disturbance downstream from ports: 20 inches, (2.3 D) 27
 Minimum number of points for velocity (nonparticulate) traverses: 12/6 3.5
 Minimum number of points for particulate traverses: 18/20
 Inside diameter of the duct: 8.00 inches 7.75
 Number of traverse points to be used on a diameter: 8
 Length of port from reference point to inside surface of duct: 6.00 inches 2.75
 Cross sectional area of sampling location: 0.349 ft² 0.328

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	6.3%	6.50
2	14.6%	7.17
3	29.6%	8.37
4	70.4%	11.63
5	85.4%	12.83
6	93.8%	13.50
↓ 8		

3.25
 3.56
 4.25
 5.25
 8.00
 9.00
 9.69
 10.00



Horizontal Duct - Flow Away From Observer

Comments: Note that the FTIR and THC sampling is conducted in this cross section. Duct location and accessibility do not provide adequate measurement conditions. Flow measurements are made before and after pollutant sampling through the single port. One traverse is used because flow rate is very low and velocity variation across the duct is not significant enough to affect representativeness of the measurements.

40 CFR 60, APPENDIX A, METHOD 1 - LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT

MRI Project No. 3804.21.04.03
 Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas
 Sampling Location: Coater Vent E10S for APP Line (E7)
 Date: 09/25/97
 Measured by J. Surman

Port - NE

Inside of far wall to outside reference point (distance Li): 35.000 inches *32 1/8*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
 Duct inside diameter (Li - Lo): 29.000 inches *28.75*

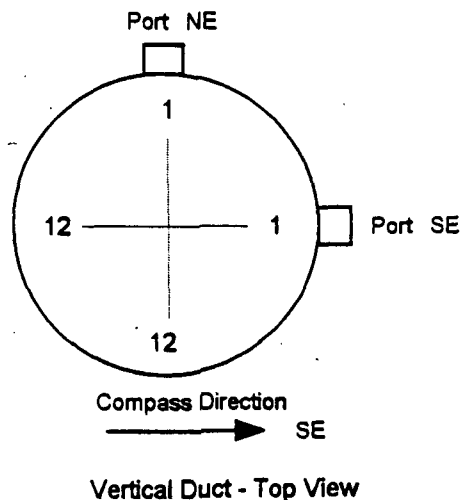
Port - SE

Inside of far wall to outside reference point (distance Li): 35.000 inches *32.38*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
 Duct inside diameter (Li - Lo): 29.000 inches *29.125* *5.7*
 Nearest flow disturbance upstream from ports: 110 inches, (*3.8 D*) *166*
 Nearest flow disturbance downstream from ports: 102 inches, (*3.8 D*) *54.5*
 Minimum number of points for velocity (nonparticulate) traverses: 18 ✓ *1.9*
 Minimum number of points for particulate traverses: *2420*

Inside diameter of the duct: 29.00 inches
 Number of traverse points to be used on a diameter: *12* *10*
 Length of port from reference point to inside surface of duct: *6.00* inches *3.25*
 Cross sectional area of sampling location: 4.587 ft² ✓

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	3.4%	7.00
2	6.7%	7.94
3	11.8%	9.43
4	17.7%	11.14
5	25.0%	13.25
6	35.6%	16.31
7	64.4%	24.69
8	75.0%	27.75
9	82.3%	29.86
10	88.2%	31.57
11	93.3%	33.06
12	96.6%	34.00

4.25
5.62
7.50
9.81
13.16
22.34
25.69
28.83
29.88
31.25



Comments: Note that the sampling location for FTIR and THC is 12 inches below (upstream from) this cross section.

**40 CFR 60, APPENDIX A, METHOD 1 -
LOCATION OF TRAVERSE POINTS IN A CIRCULAR DUCT**

MRI Project No. 3804.21.04.03:

Client/Source: U.S. EPA-EMC / U.S. Intec, Inc., Port Arthur, Texas

Sampling Location: Coater Vent E20S for SBS Line (E8)

Date: 09/25/97

Measured by J. Surman

Port - NE

Inside of far wall to outside reference point (distance Li): 35.000 inches *32 1/8*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
 Duct inside diameter (Li - Lo): 29.000 inches *28.875*

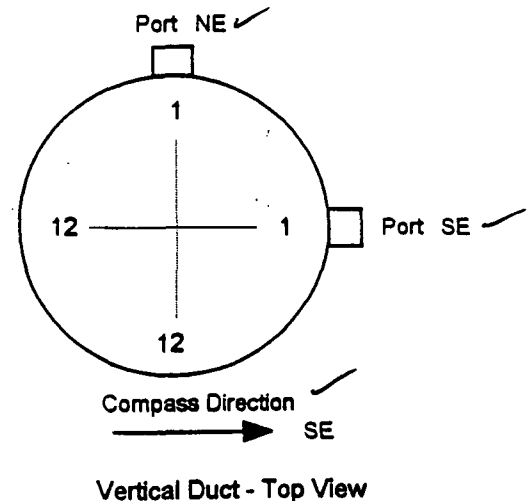
Port - SE

Inside of far wall to outside reference point (distance Li): 35.000 inches *32 3/8*
 Inside of near wall to outside reference point (distance Lo): 6.000 inches *3.25*
 Duct inside diameter (Li - Lo): 29.000 inches *29.125 (6.1)*
 Nearest flow disturbance upstream from ports: 110 inches, (*3.8 D*) *176*
 Nearest flow disturbance downstream from ports: 102 inches, (*3.5 D*) *65*
 Minimum number of points for velocity (nonparticulate) traverses: *18/2* *2.2*
 Minimum number of points for particulate traverses: *24/6*

Inside diameter of the duct: 29.00 inches
 Number of traverse points to be used on a diameter: *12/8*
 Length of port from reference point to inside surface of duct: *6.00* inches *3.25*
 Cross sectional area of sampling location: 4.587 ft²

Traverse Point	Percent of Duct Diameter from Wall to Traverse Point	Distance from Reference Point to Traverse Point, inches
1	3.4%	7.00
2	6.7%	7.94
3	11.8%	9.43
4	17.7%	11.14
5	25.0%	13.25
6	35.6%	16.31
7	64.4%	24.69
8	75.0%	27.75
9	82.3%	29.86
10	88.2%	31.57
11	93.3%	33.06
12	96.6%	34.00

4.25
6.29
9.87
12.62
22.88
26.63
29.21
31.25



Comments: Note that the sampling location for FTIR and THC is 12 inches below (upstream from) this cross section.

FTIR FIELD DATA FORM
Sampling Location Data

PROJECT NO. 3804-21-04-03

BAROMETRIC: 29.98

PLANT: US INTER, GAF

DATE: 9/22/97

OPERATOR: Klamm & Edwards

INLET					
SAMPLE TIME	DELTA P IN. H2O	STACK TEMP.	PROBE TEMP.	FILTER TEMP.	
1450	0.01	95	301	303	START
1505	0.01	94	300	301	
1520	0.01	98	303	303	
1535	0.01	98	302	301	
1550	0.01	97	301	303	
1605	0.01	96	300	302	
1620	0.01	86	300	302	Rain
1635	0.01	90	300	305	
1650	0.01	92	301	304	Art Change
1725	0.01	91	303	303	Restart
1740	0.01	87	300	302	
1755	0.01	89	299	303	
1820	0.01	90	300	304	
1835	0.01	90	301	304	
1850	0.01	90	300	303	
1905	0.01	90	302	299	
1925	0.01	90	302	299	

OUTLET					
SAMPLE TIME	DELTA P IN. H2O	STACK TEMP.	PROBE TEMP.	FILTER TEMP.	
"	0.16	419	304	304	
"	0.16	419	301	302	
"	0.15	420	298	304	
"	0.15	419	300	303	
"	0.155	422	304	304	
"	0.155	420	304	302	
"	0.16	413	303	304	
"	0.15	414	301	304	
"	0.15	416	298	304	
"	0.16	417	302	304	
"	0.15	416	301	304	
"	0.16	416	302	304	
"	0.16	416	302	305	
"	0.155	417	303	305	
"	0.16	410	303	304	
"	0.15	420	301	304	
"	0.15	420	300	301	

PROJECT NO. 3804-21-04-03

PLANT: US INTER GAF

DATE: 9/23/97

BAROMETRIC: 29.92

OPERATOR: Mumm & Edwards

[illegible]

FTIR FIELD DATA FORM

Sampling Location Data

PROJECT NO. 3804-21-04-03BAROMETRIC: 29.84PLANT: US INTEL GAFDATE: 9/23/97OPERATOR: Klamm + Edwards

INLET					
SAMPLE TIME	DELTA P IN. H ₂ O	STACK TEMP.	PROBE TEMP.	FILTER TEMP.	
1710	0.01	88	298	303	
1725	0.01	90	303	304	
1740	0.01	90	302	303	
1755	0.01	89	301	303	
1810	0.01	90	304	303	
1825	0.01	90	298	302	
1840	0.01	90	299	303	
1855	0.01	90	303	303	
1910	0.01	89	301	303	Port Change
1935	0.01	89	299	301	Restart
1950	0.01	88	302	298	
2005	0.01	88	302	299	
2020	0.01	87	300	299	
2035	0.01	87	303	300	
2050	0.01	87	303	300	
2105	0.01	87	302	303	
2120	0.01	88	300	304	
2135	0.01	87	301	302	

OUTLET					
SAMPLE TIME	DELTA P IN. H ₂ O	STACK TEMP.	PROBE TEMP.	FILTER TEMP.	
1710	0.15	418	305	304	
1725	0.16	418	304	305	
1740	0.16	418	305	304	
1755	0.15	418	306	304	
1810	0.15	420	301	304	
1825	0.16	418	301	304	
1840	0.15	418	299	304	
1855	0.15	414	304	303	
1910	0.15	414	305	304	
1935	0.15	417	304	304	
1950	0.16	418	299	304	
2005	0.155	418	304	305	
2020	0.15	416	302	304	
2035	0.15	416	301	304	
2050	0.15	416	303	304	
2105	0.15	417	299	304	
2120	0.15	417	299	304	
2135	0.15	417	302	304	

FTIR FIELD DATA FORM

BAROMETRIC: 29.85

DATE: 9/24/97

OPERATOR: Klamm & Edwards

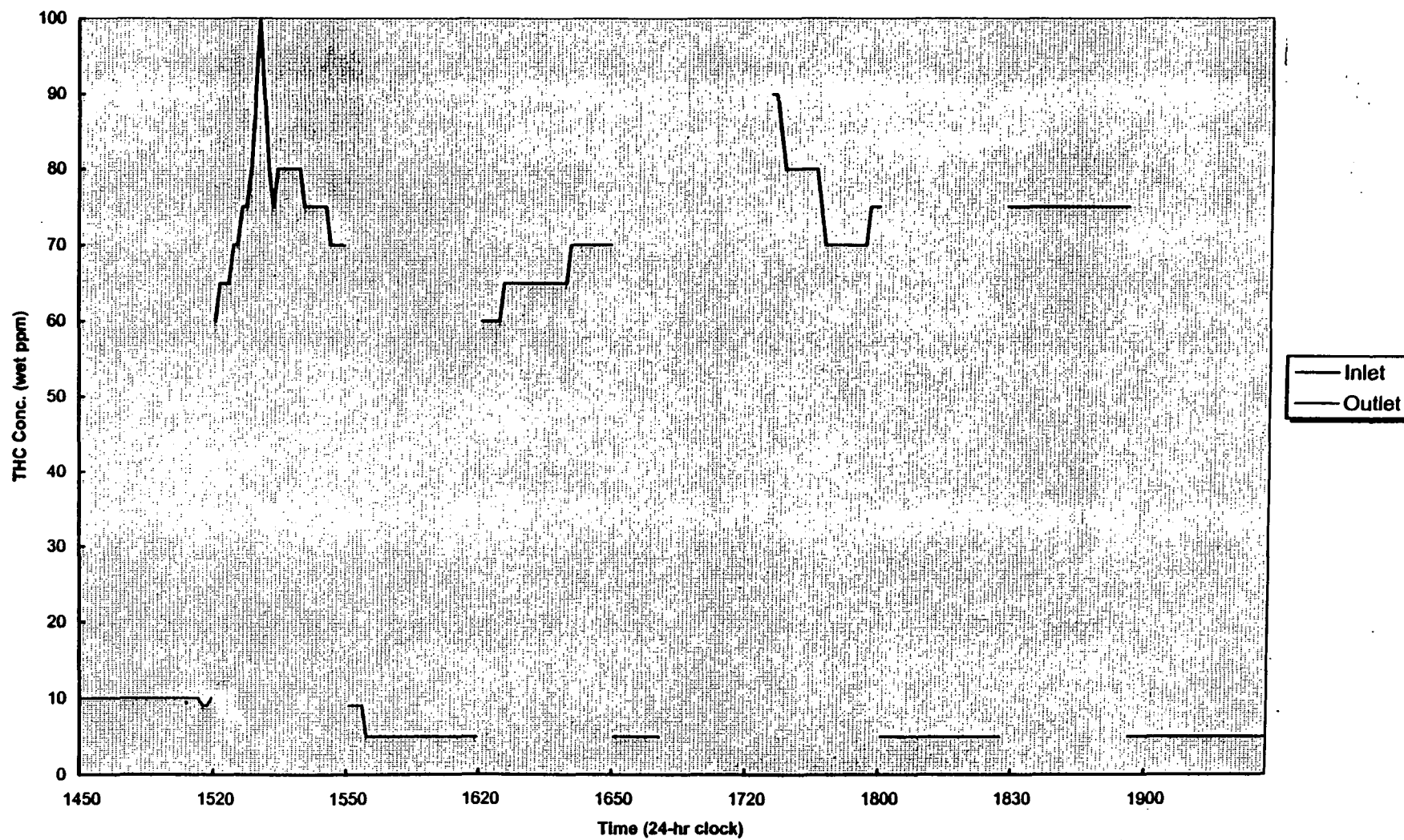
~~INLET~~ APP 1

~~OUTLET~~ SBS 2

APPENDIX B
THC ANALYZER DATA

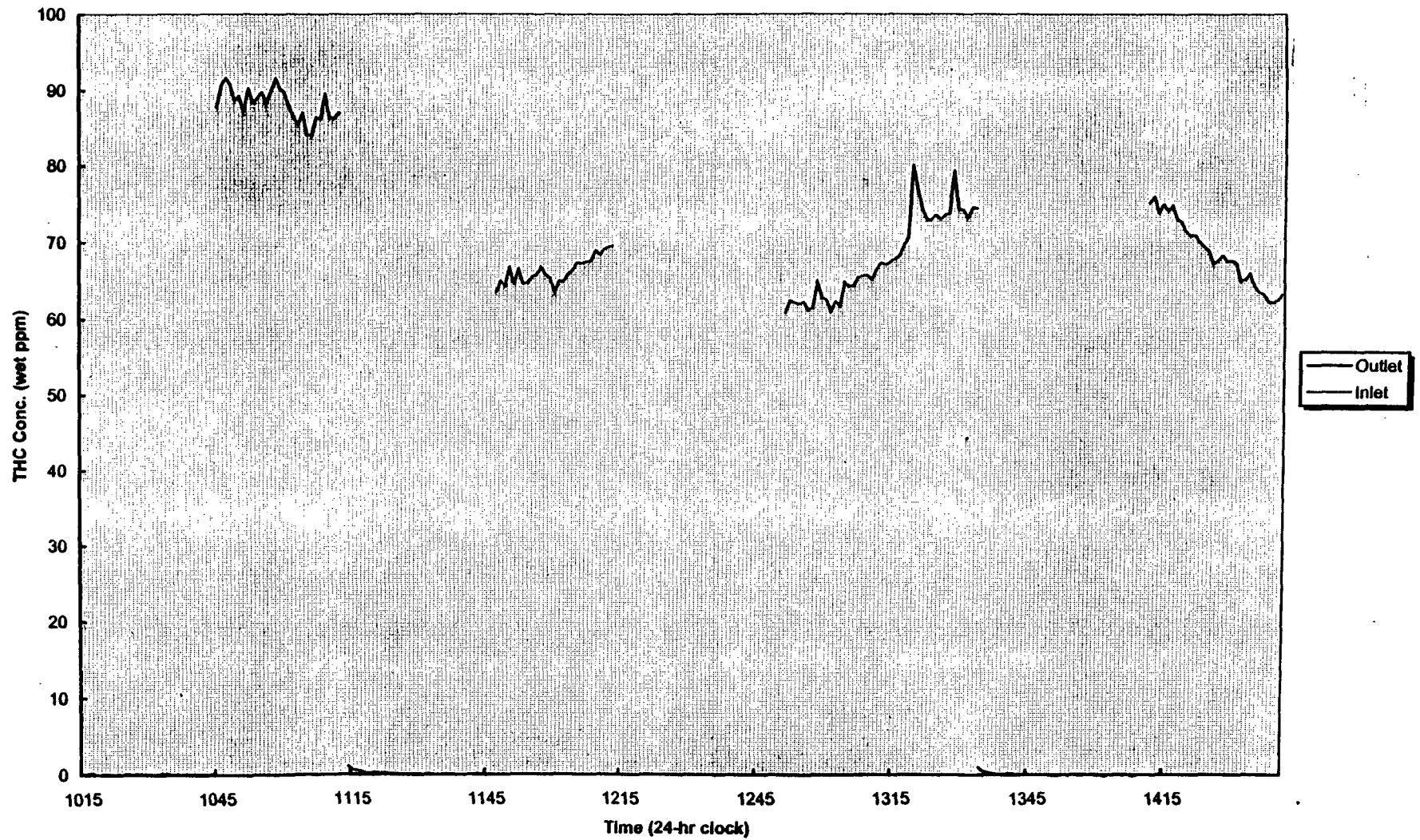
Run1TO Chart 1

Run 1 Thermal Oxidizer Inlet/Outlet



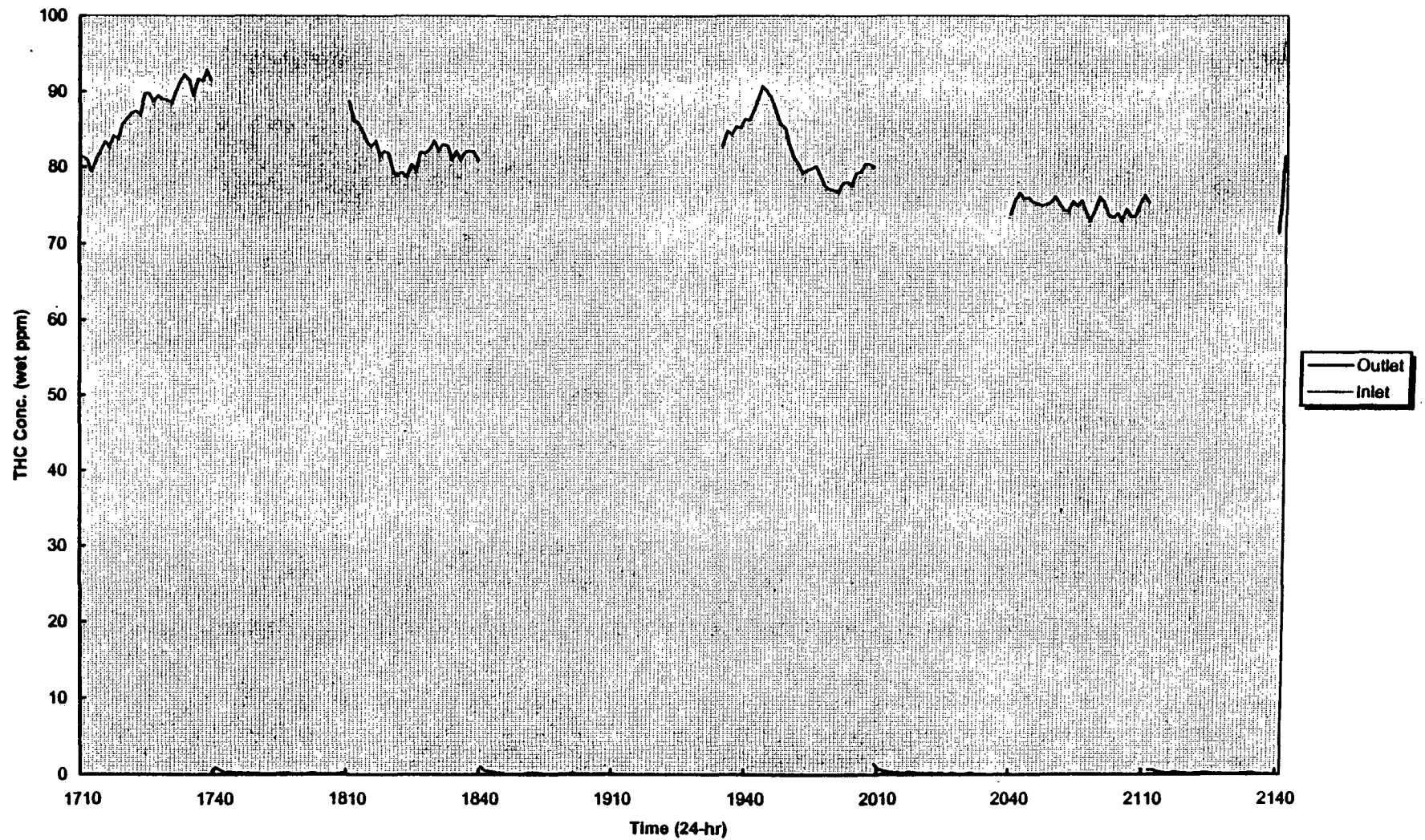
A Chart 1

Run 2 Thermal Oxidizer Inlet/Outlet



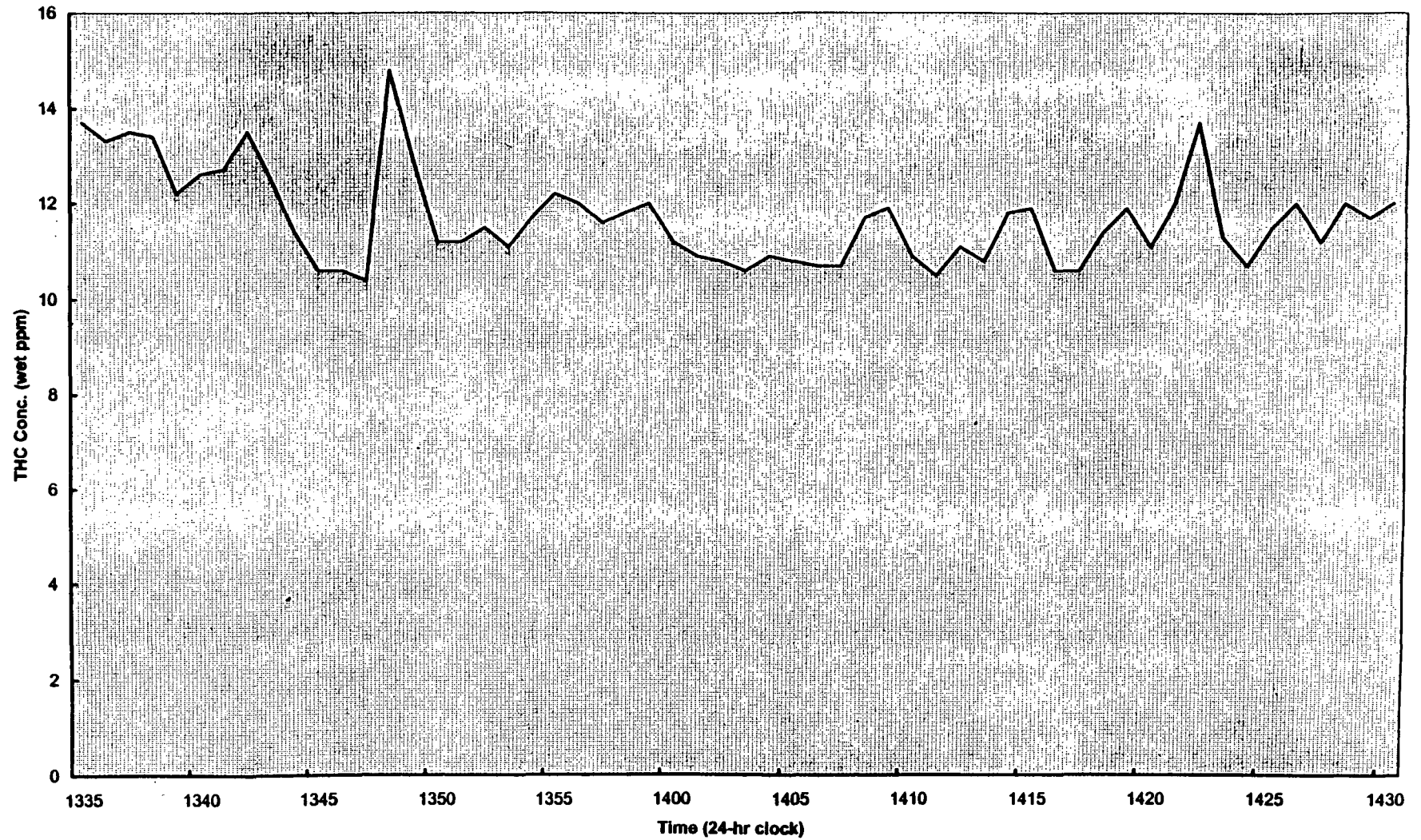
A Chart 2

Run 3 Thermal Oxidizer Inlet/Outlet



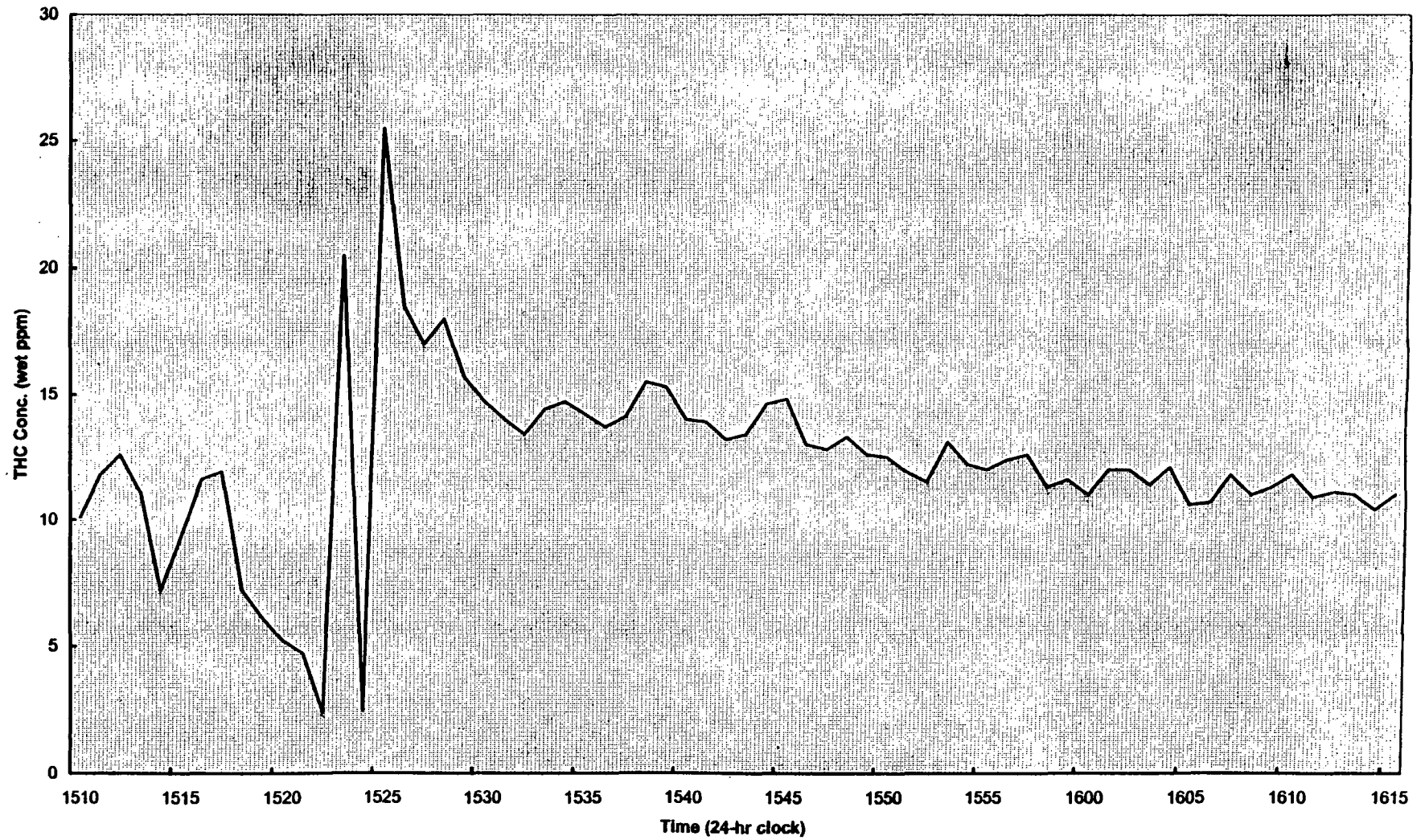
A Chart 1

Run 1 APP Coater Roof Stack



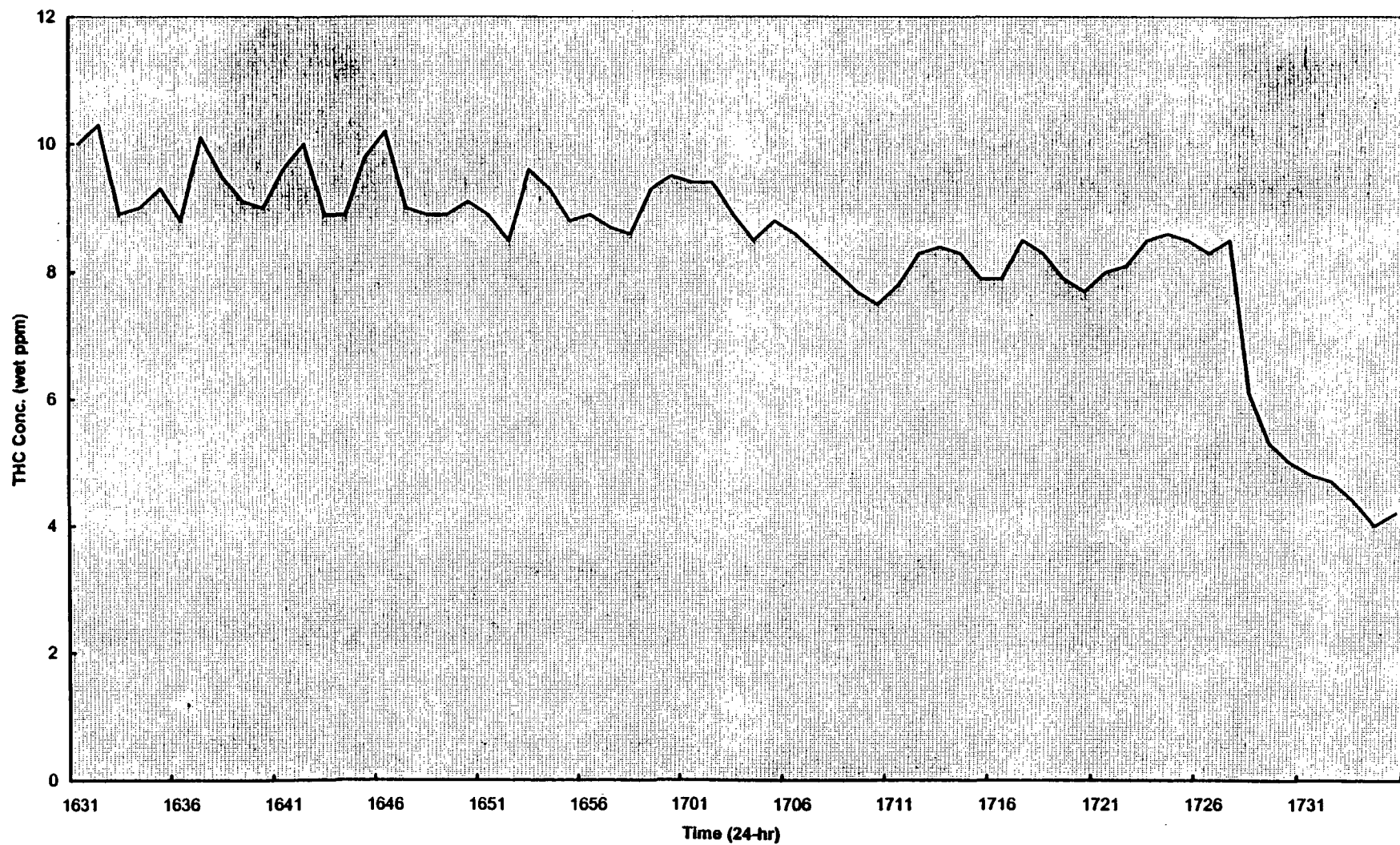
A Chart 1

Run 2 APP Coater Roof Stack



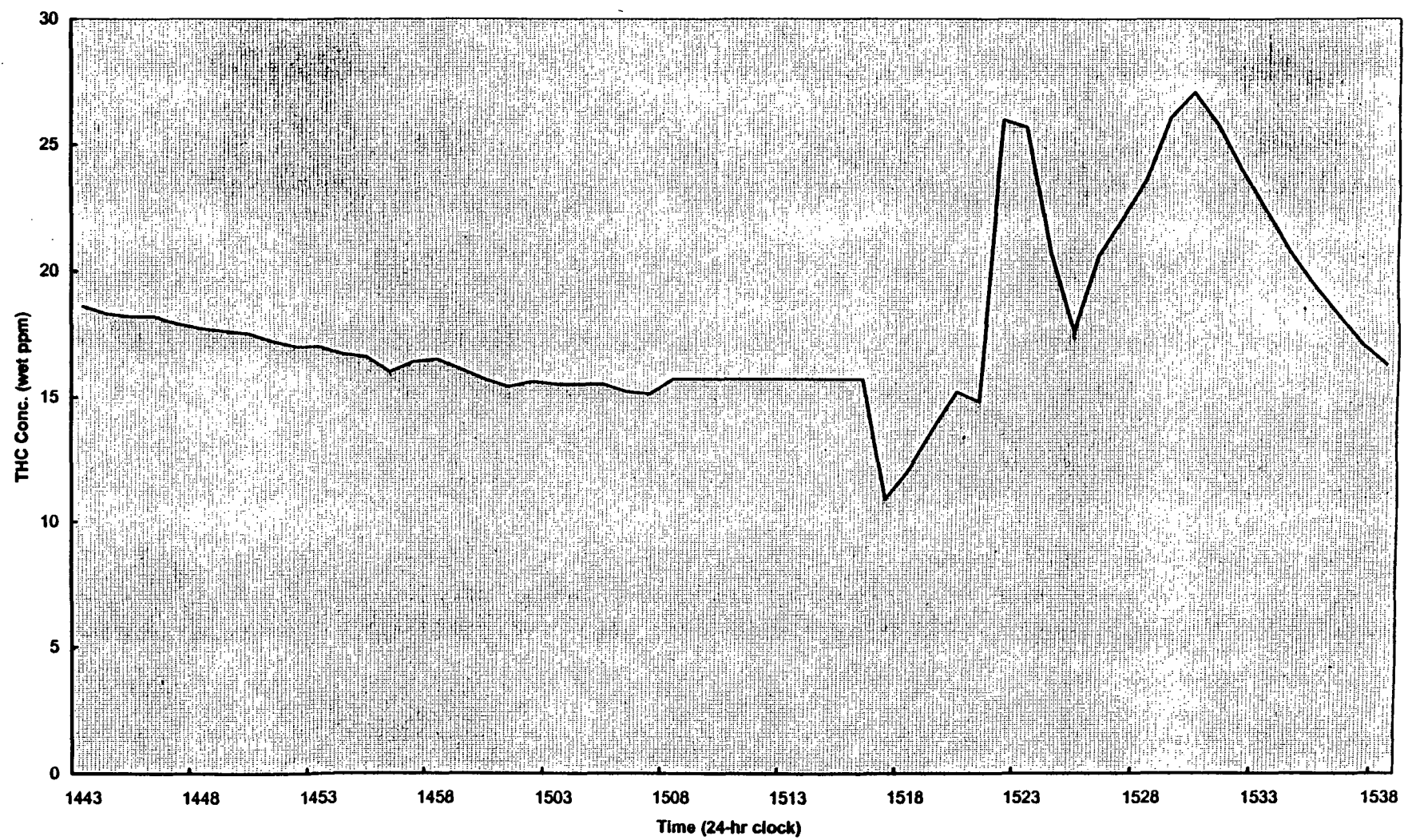
A Chart 1

Run 3 APP Coater Roof Stack



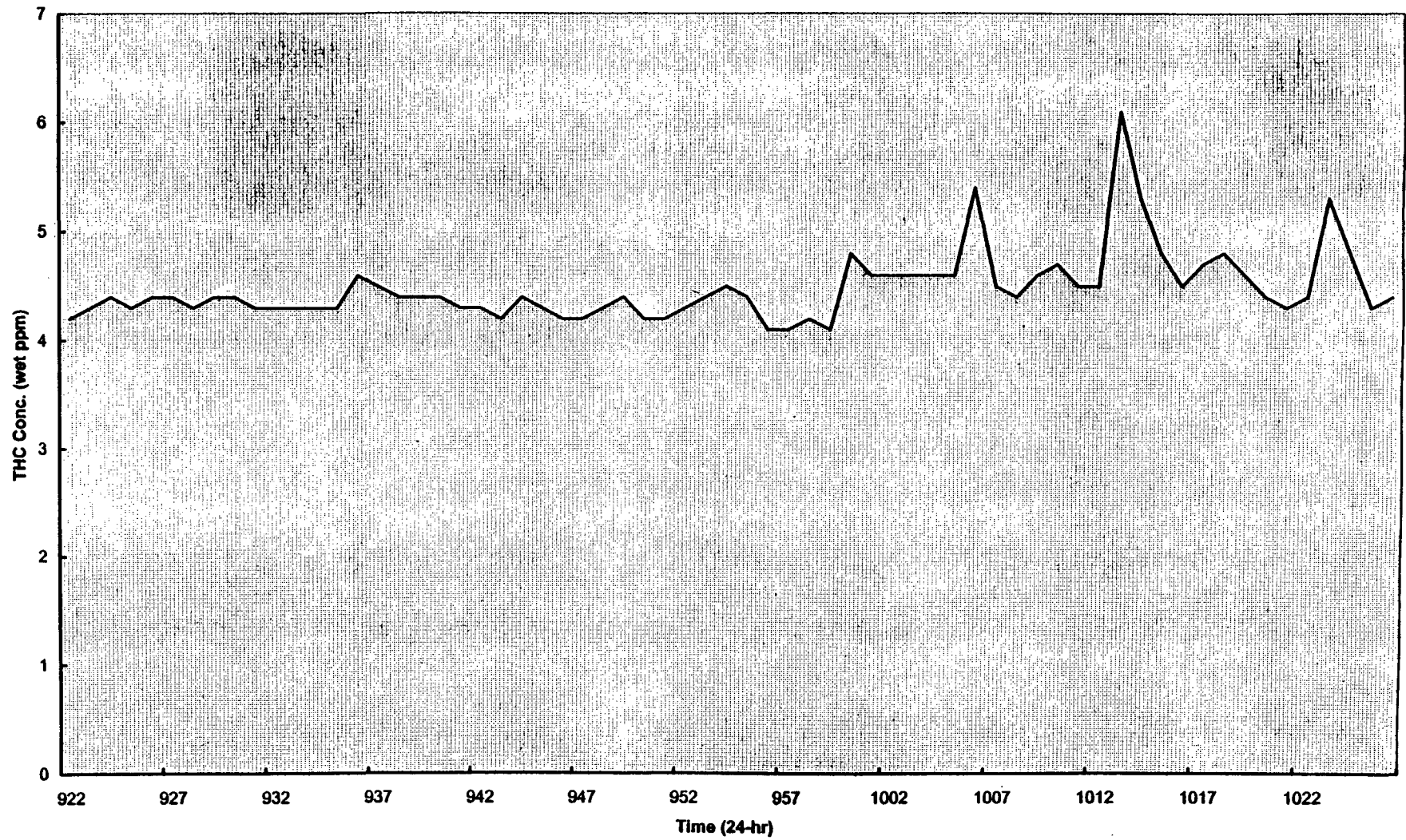
A Chart 1

Run 1 SBS Coater Roof Stack



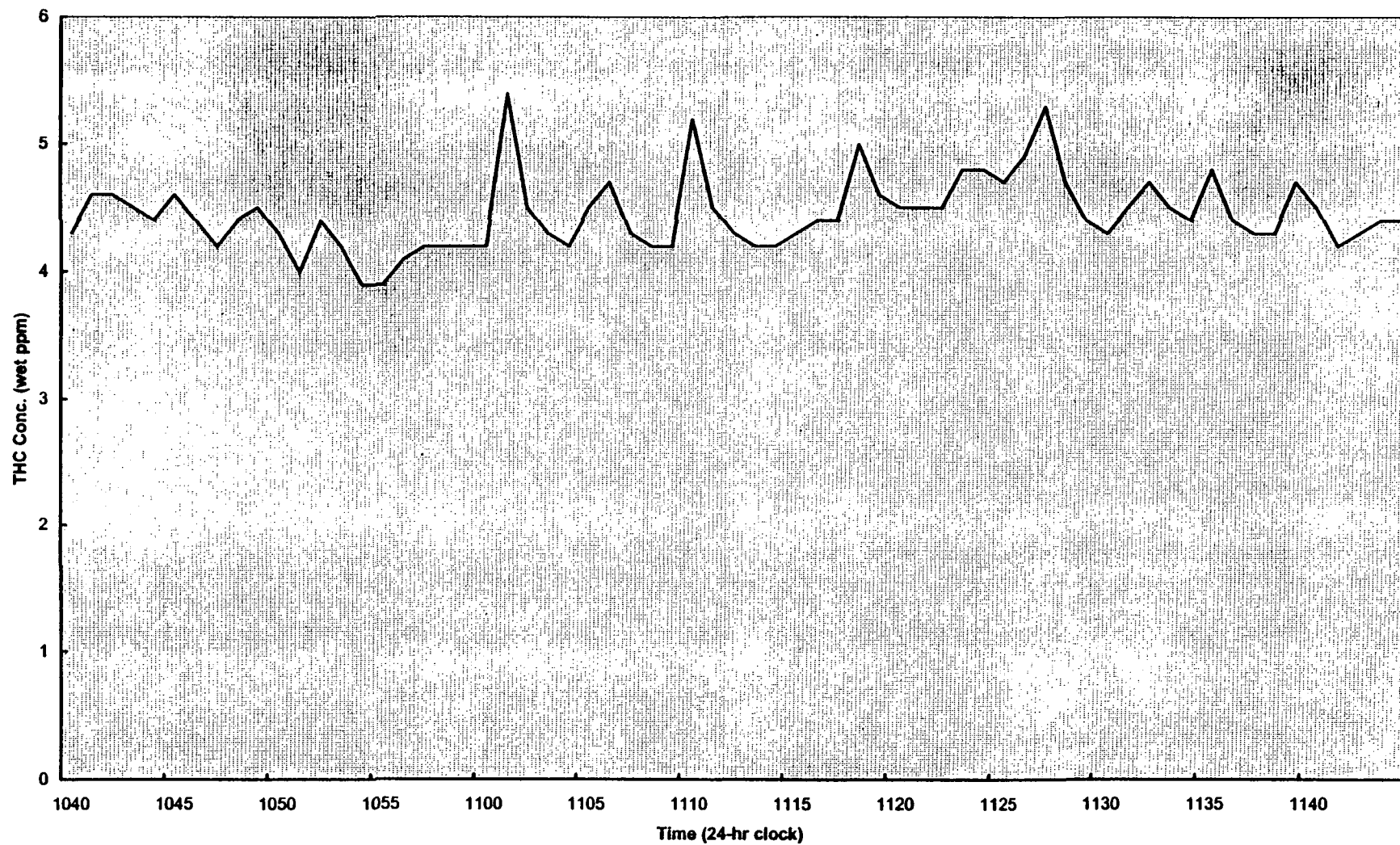
A Chart 1

Run 2 SBS Coater Roof Stack



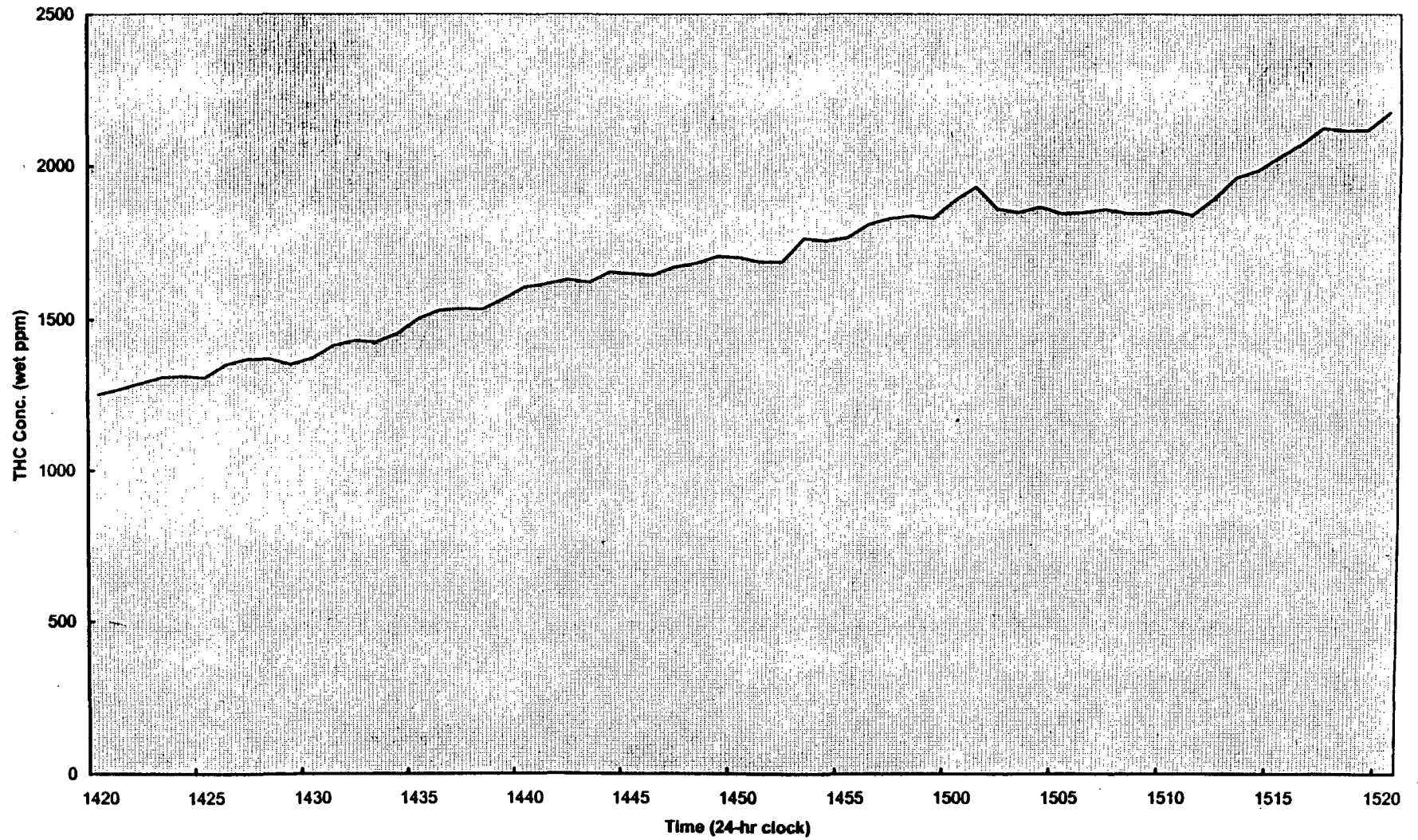
A Chart 1

Run 3 SBS Coater Roof Stack



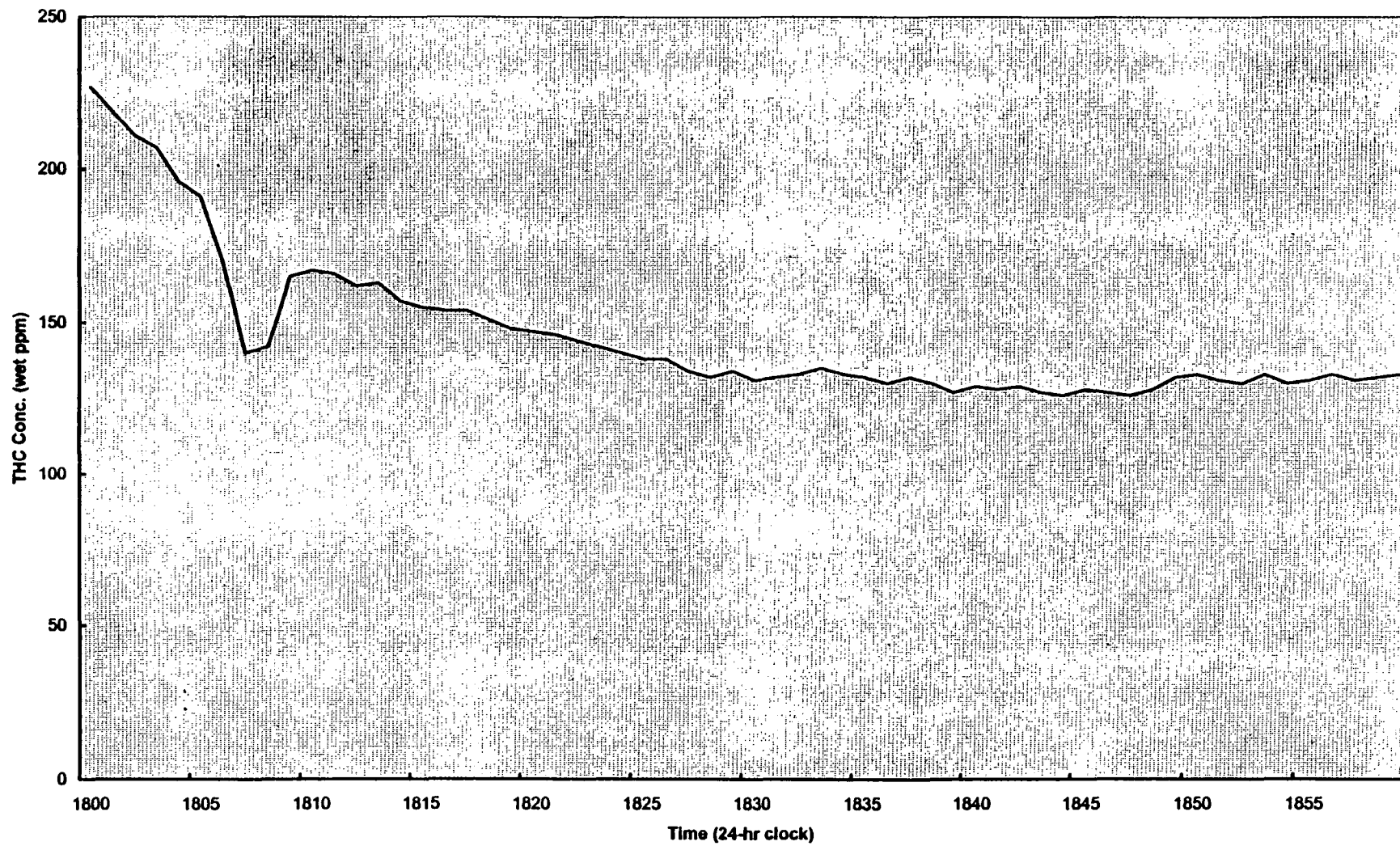
A Chart 1

APP Mixing Tank 1



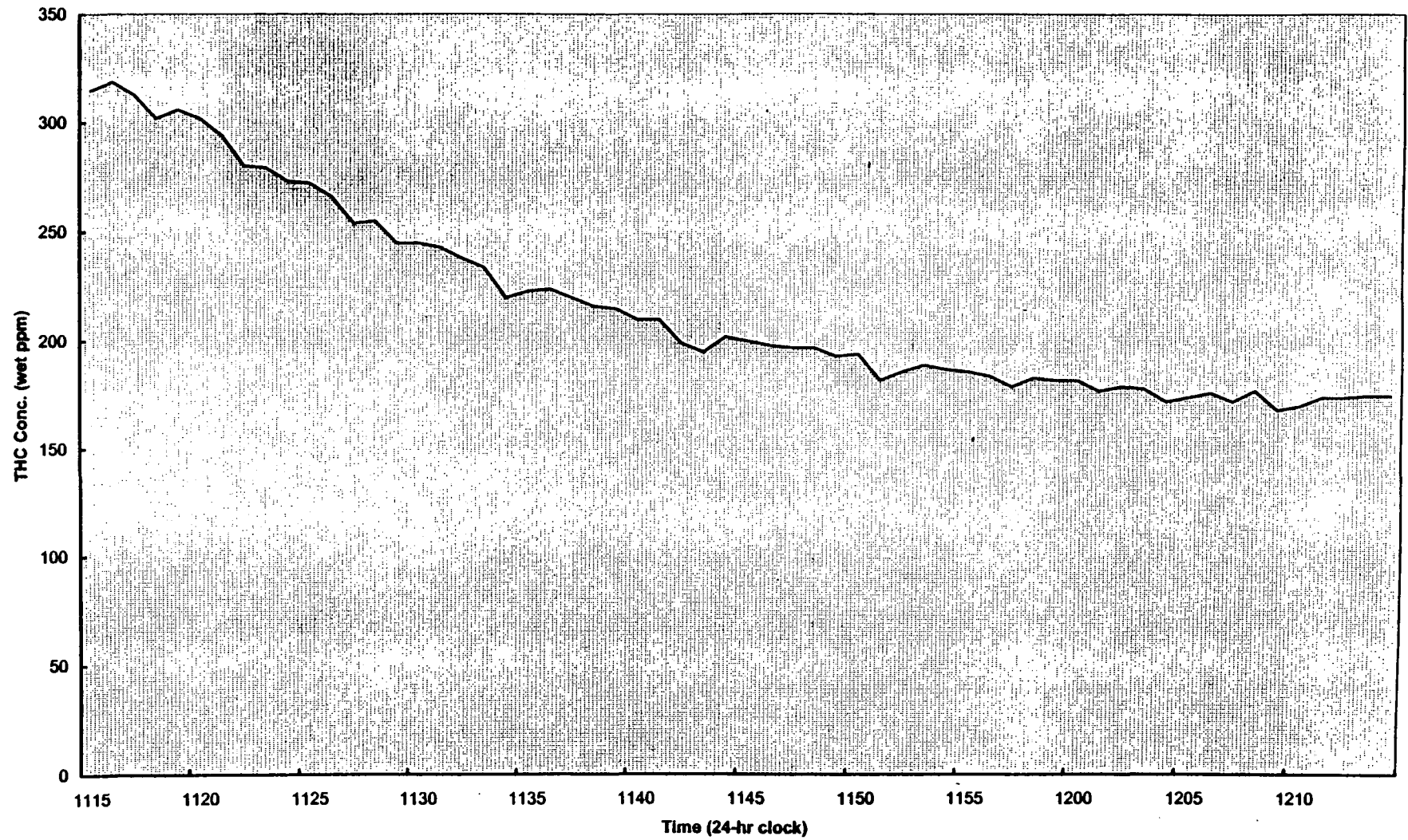
A Chart 1

SBS Mixing Tank 11



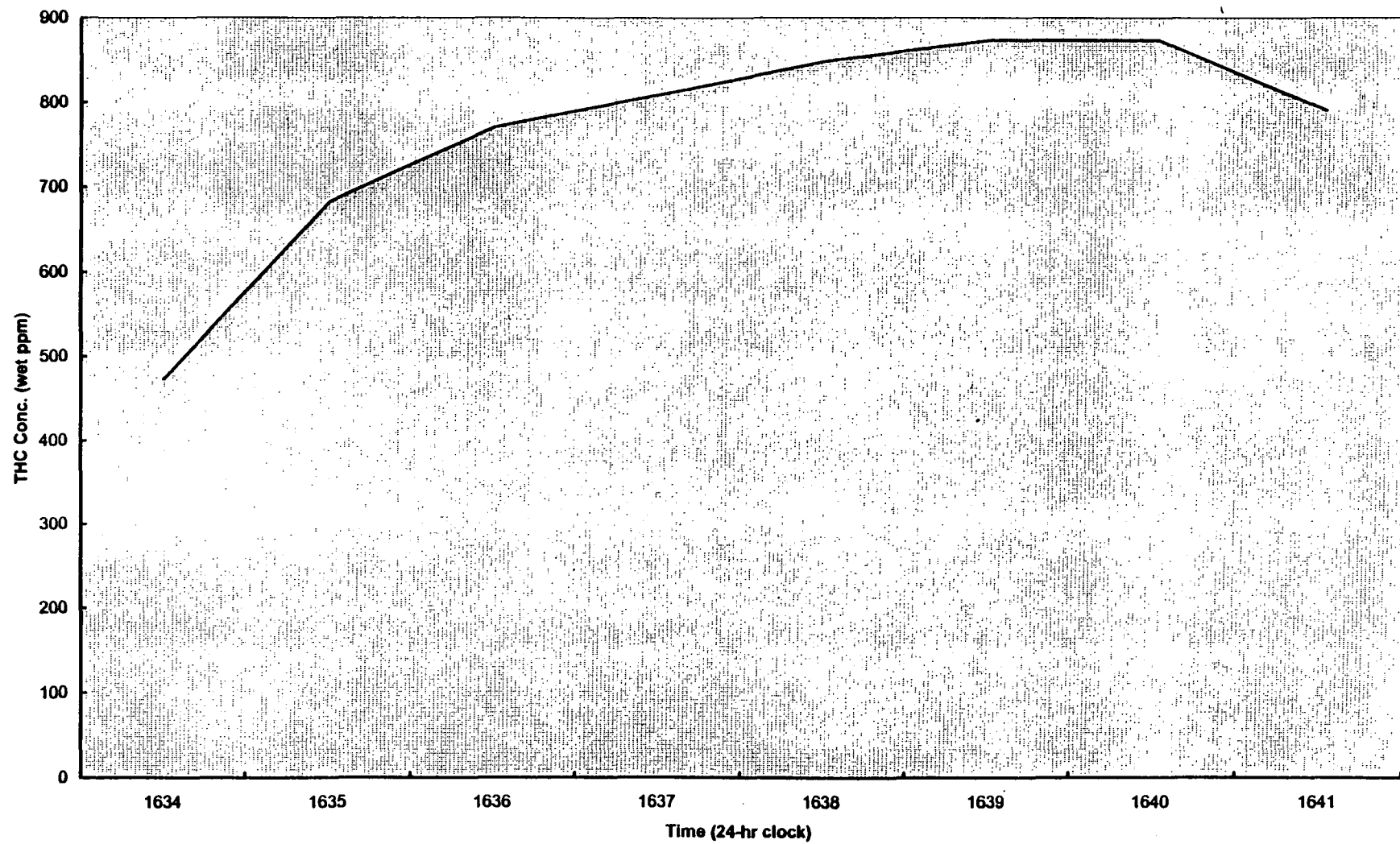
A Chart 1

SBS Holding Tank 3



A Chart 1

APP Holding Tank 1



U.S. Intec
Run 1 Thermal Oxidizer
Date 9/22/97
Operator: Gulick

Time (24 hr)	THC Inlet (ppm) Inlet	THC Outlet (ppm) Outlet
1450		10
1451		10
1452		10
1453		10
1454		10
1455		10
1456		10
1457		10
1458		10
1459		10
1500		10
1501		10
1502		10
1503		10
1504		10
1505		10
1506		10
1507		10
1508		10
1509		10
1510		10
1511		10
1512		10
1513		10
1514		10
1515		10
1516		10
1517		9
1518		9
1519		10
1520	60	
1521	65	
1522	65	
1523	65	
1524	70	
1525	70	
1526	75	
1527	75	
1528	80	

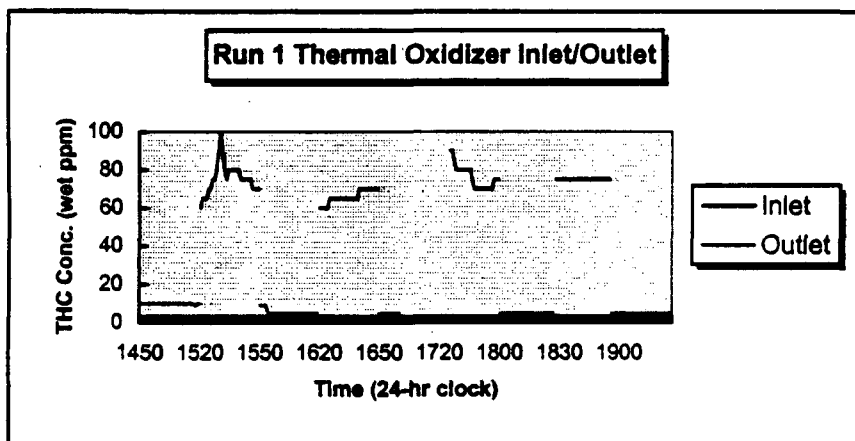
1529	90	
1530	100	
1531	90	
1532	80	
1533	75	
1534	80	
1535	80	
1536	80	
1537	80	
1538	80	
1539	80	
1540	75	
1541	75	
1542	75	
1543	75	
1544	75	
1545	75	
1546	70	
1547	70	
1548	70	
1549	70	
1550		9
1551		9
1552		9
1553		9
1554		5
1555		5
1556		5
1557		5
1558		5
1559		5
1600		5
1601		5
1602		5
1603		5
1604		5
1605		5
1606		5
1607		5
1608		5
1609		5
1610		5
1611		5
1612		5
1613		5
1614		5
1615		5
1616		5

1617		5
1618		5
1619		5
1620	60	
1621	60	
1622	60	
1623	60	
1624	60	
1625	65	
1626	65	
1627	65	
1628	65	
1629	65	
1630	65	
1631	65	
1632	65	
1633	65	
1634	65	
1635	65	
1636	65	
1637	65	
1638	65	
1639	65	
1640	70	
1641	70	
1642	70	
1643	70	
1644	70	
1645	70	
1646	70	
1647	70	
1648	70	
1649	70	
1650		5
1651		5
1652		5
1653		5
1654		5
1655		5
1656		5
1657		5
1658		5
1659		5
1700		5
1701		
1702		
1703		
1704		

1705		
1706		
1707		
1708		
1709		
1710		
1711		
1712		
1713		
1714		
1715		
1716		
1717		
1718		
1719		
1720		
1721		
1722		
1723		
1724		
1725	90	
1726	90	
1727	85	
1728	80	
1729	80	
1730	80	
1731	80	
1732	80	
1733	80	
1734	80	
1735	80	
1736	75	
1737	70	
1738	70	
1739	70	
1740	70	
1741	70	
1742	70	
1743	70	
1744	70	
1745	70	
1746	70	
1747	75	
1748	75	
1749	75	
1800		5
1801		5
1802		5

1803		5
1804		5
1805		5
1806		5
1807		5
1808		5
1809		5
1810		5
1811		5
1812		5
1813		5
1814		5
1815		5
1816		5
1817		5
1818		5
1819		5
1820		5
1821		5
1822		5
1823		5
1824		5
1825		5
1826		5
1827		5
1828	75	
1829	75	
1830	75	
1831	75	
1832	75	
1833	75	
1834	75	
1835	75	
1836	75	
1837	75	
1838	75	
1839	75	
1840	75	
1841	75	
1842	75	
1843	75	
1844	75	
1845	75	
1846	75	
1847	75	
1848	75	
1849	75	
1850	75	

1851	75	
1852	75	
1853	75	
1854	75	
1855	75	
1856		5
1857		5
1858		5
1859		5
1900		5
1901		5
1902		5
1903		5
1904		5
1905		5
1906		5
1907		5
1908		5
1909		5
1910		5
1911		5
1912		5
1913		5
1914		5
1915		5
1916		5
1917		5
1918		5
1919		5
1920		5
1921		5
1922		5
1923		5
1924		5
1925		5
1926		5



U.S. Intec
Run 2 Thermal Oxidizer
Date 9/23/97
Operator: Gulick

Time (24 hr)	THC Outlet (ppm)	THC Inlet (ppm)
Time (24-hr)	Outlet	Inlet
1015	0.1	
1016	0.1	
1017	0.2	
1018	0.0	
1019	0.0	
1020	0.1	
1021	0.1	
1022	0.0	
1023	0.1	
1024	0.0	
1025	0.1	
1026	0.0	
1027	0.1	
1028	0.1	
1029	0.1	
1030	0.1	
1031	0.0	
1032	0.1	
1033	0.2	
1034	0.1	
1035	0.0	
1036	0.1	
1037	0.0	
1038	0.1	
1039	0.0	
1040	0.1	
1041	0.1	
1042	0.1	
1043	0.1	
1044	0.1	
1045		87.8
1046		90.8
1047		91.7
1048		90.8
1049		88.7
1050		89.3
1051		87.3
1052		90.3

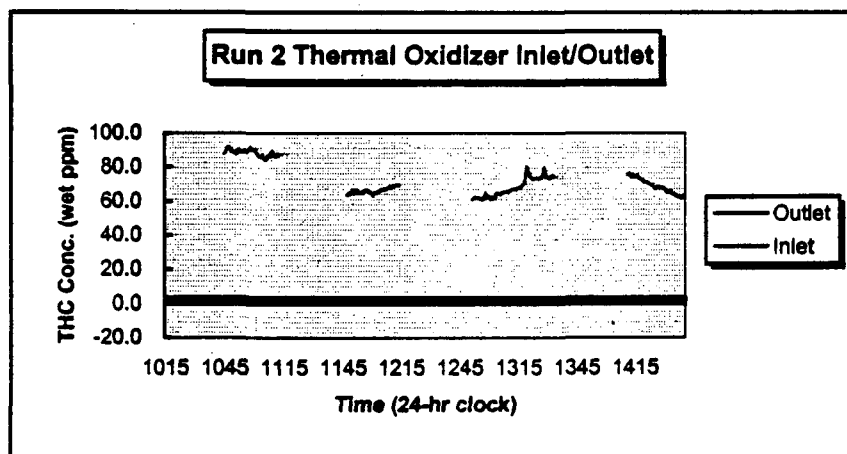
1053		88.4
1054		89.1
1055		89.8
1056		88.3
1057		89.9
1058		91.7
1059		90.3
1100		89.8
1101		88.1
1102		86.5
1103		85.5
1104		87.1
1105		84.1
1106		84.0
1107		86.5
1108		86.2
1109		89.7
1110		86.4
1111		86.3
1112		87.1
1113		
1114	1.1	
1115	0.6	
1116	0.5	
1117	0.4	
1118	0.2	
1119	0.2	
1120	0.3	
1121	0.2	
1122	0.2	
1123	0.1	
1124	0.1	
1125	0.1	
1126	0.0	
1127	0.1	
1128	0.1	
1129	0.1	
1130	0.1	
1131	0.0	
1132	0.1	
1133	0.0	
1134	0.0	
1135	0.0	
1136	0.1	
1137	0.1	
1138	0.0	
1139	0.0	
1140	0.0	

1141	0.0	
1142	0.0	
1143	0.1	
1144	0.0	
1145	-0.1	
1146	0.0	
1147		63.7
1148		65.1
1149		64.4
1150		66.9
1151		64.6
1152		66.7
1153		64.7
1154		64.8
1155		65.6
1156		65.8
1157		66.9
1158		65.9
1159		65.3
1200		63.6
1201		65.0
1202		65.0
1203		65.9
1204		66.4
1205		67.4
1206		67.3
1207		67.5
1208		67.6
1209		69.0
1210		68.5
1211		69.2
1212		69.4
1213		69.6
1214	Port Change	
1215	"	
1216	"	
1217	"	
1218	"	
1219	"	
1220	"	
1221	"	
1222	"	
1223	"	
1224	"	
1225	"	
1226	"	
1227	"	
1228	"	

1229	"	
1230	"	
1231	"	
1232	"	
1233	"	
1234	"	
1235	"	
1236	"	
1237	"	
1238	"	
1239	"	
1240	Off Line	
1241	"	
1242	"	
1243	"	
1244	"	
1245	"	
1246	"	
1247	"	
1248	"	
1249	"	
1250	"	
1251		60.9
1252		62.5
1253		62.2
1254		62.0
1255		62.3
1256		61.2
1257		61.5
1258		65.1
1259		62.8
1300		62.6
1301		61.1
1302		62.4
1303		61.8
1304		65.0
1305		64.3
1306		64.4
1307		65.5
1308		65.7
1309		65.8
1310		65.2
1311		66.6
1312		67.4
1313		67.2
1314		67.5
1315		67.9
1316		68.3

1317		69.8
1318		70.7
1319		80.1
1320		77.3
1321		74.4
1322		73.1
1323		73.0
1324		73.6
1325		73.1
1326		73.6
1327		73.8
1328		79.4
1329		74.3
1330		74.3
1331		73.2
1332		74.6
1333		74.4
1334	1.0	
1335	0.5	
1336	0.3	
1337	0.2	
1338	0.1	
1339	0.1	
1340	0.1	
1341	0.2	
1342	0.1	
1343	0.1	
1344	0.1	
1345	0.0	
1346	0.0	
1347	0.0	
1348	0.0	
1349	0.0	
1350	-0.1	
1351	-0.1	
1352	-0.1	
1353	0.0	
1354	-0.1	
1355	0.0	
1356	-0.1	
1357	-0.1	
1358	0.0	
1359	0.0	
1400	-0.1	
1401	-0.1	
1402	-0.2	
1403	0.0	
1404	-0.1	

1405	0.0
1406	-0.1
1407	0.0
1408	-0.2
1409	-0.1
1410	
1411	75.2
1412	76.0
1413	73.9
1414	75.0
1415	74.1
1416	74.9
1417	73.1
1418	72.7
1419	71.5
1420	70.9
1421	71.0
1422	70.0
1423	69.5
1424	68.9
1425	67.2
1426	67.7
1427	68.4
1428	67.6
1429	67.7
1430	67.3
1431	64.9
1432	65.3
1433	66.0
1434	64.2
1435	63.5
1436	63.3
1437	62.3
1438	62.2
1439	62.5
1440	63.2



U.S. Intec
Run 3 Thermal Oxidizer
Date: 9/23/97
Operator: Gulick

Time (24 hr)	THC Outlet (ppm)	THC Inlet (ppm)
	Outlet	Inlet
1710		81.3
1711		81.0
1712		79.4
1713		80.9
1714		82.1
1715		83.3
1716		82.6
1717		84.1
1718		83.7
1719		85.7
1720		86.3
1721		87.2
1722		87.4
1723		87.0
1724		89.7
1725		89.8
1726		88.7
1727		89.5
1728		89.0
1729		88.9
1730		88.5
1731		90.1
1732		91.4
1733		92.3
1734		91.6
1735		89.6
1736		91.7
1737		91.4
1738		92.9
1739		91.6
1740	0.9	
1741	0.6	
1742	0.3	
1743	0.3	
1744	0.3	
1745	0.2	
1746	0.2	
1747	0.2	
1748	0.2	

1749	0.2	
1750	0.1	
1751	0.1	
1752	0.1	
1753	0.1	
1754	0.1	
1755	0.2	
1756	0.2	
1757	0.1	
1758	0.1	
1759	0.1	
1800	0.1	
1801	0.1	
1802	0.2	
1803	0.1	
1804	0.1	
1805	0.1	
1806	0.1	
1807	0.0	
1808	0.1	
1809	0.2	
1810		88.8
1811		86.3
1812		85.8
1813		84.8
1814		83.4
1815		82.7
1816		83.5
1817		81.5
1818		82.1
1819		81.8
1820		79.3
1821		79.0
1822		79.3
1823		78.7
1824		80.4
1825		79.6
1826		82.0
1827		81.8
1828		82.3
1829		83.5
1830		82.2
1831		83.0
1832		82.8
1833		81.1
1834		82.1
1835		81.0
1836		82.0

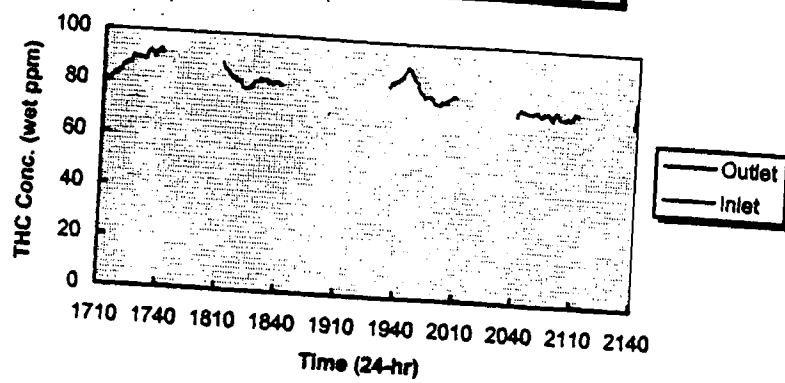
1837		82.1
1838		82.0
1839		80.9
1840	1.0	
1841	0.5	
1842	0.4	
1843	0.3	
1844	0.2	
1845	0.2	
1846	0.0	
1847	0.1	
1848	0.1	
1849	0.1	
1850	0.1	
1851	0.2	
1852	0.2	
1853	0.2	
1854	0.1	
1855	0.1	
1856	0.1	
1857	0.1	
1858	0.1	
1859	0.1	
1900	0.1	
1901	0.2	
1902	0.0	
1903	0.1	
1904	0.1	
1905	0.0	
1906	0.1	
1907	0.1	
1908	0.1	
1909	0.1	
1910	0.1	
1911	Port Change	
1912	"	
1913	"	
1914	"	
1915	"	
1916	"	
1917	"	
1918	"	
1919	"	
1920	"	
1921	"	
1922	"	
1923	"	
1924	"	

1925	"	
1926	"	
1927	"	
1928	"	
1929	"	
1930	"	
1931	"	
1932	"	
1933	"	
1934		82.8
1935		84.8
1936		84.3
1937		85.4
1938		85.2
1939		86.4
1940		86.2
1941		87.6
1942		89.0
1943		90.8
1944		90.1
1945		89.3
1946		87.4
1947		85.7
1948		85.2
1949		82.9
1950		81.3
1951		80.4
1952		79.2
1953		79.6
1954		79.8
1955		80.1
1956		78.8
1957		77.4
1958		77.1
1959		76.9
2000		76.7
2001		77.9
2002		78.0
2003		77.6
2004		79.2
2005		79.3
2006		80.4
2007		80.4
2008		80.0
2009	1.4	
2010	0.7	
2011	0.5	
2012	0.4	

2013	0.3	
2014	0.3	
2015	0.2	
2016	0.2	
2017	0.3	
2018	0.2	
2019	0.1	
2020	0.2	
2021	0.1	
2022	0.2	
2023	0.1	
2024	0.2	
2025	0.1	
2026	0.1	
2027	0.2	
2028	0.1	
2029	0.1	
2030	0.1	
2031	0.2	
2032	0.0	
2033	0.1	
2034	0.1	
2035	0.0	
2036	0.0	
2037	0.1	
2038	0.1	
2039		73.9
2040		75.7
2041		76.6
2042		75.8
2043		76.0
2044		75.4
2045		75.2
2046		74.9
2047		75.1
2048		75.3
2049		76.1
2050		75.2
2051		74.3
2052		74.2
2053		75.5
2054		74.9
2055		75.6
2056		74.1
2057		73.0
2058		74.5
2059		76.1
2100		75.4

2101		73.7
2102		73.4
2103		73.9
2104		73.1
2105		74.5
2106		73.6
2107		73.6
2108		75.1
2109		76.3
2110		75.4
2111	0.6	
2112	0.6	
2113	0.4	
2114	0.3	
2115	0.2	
2116	0.2	
2117	0.3	
2118	0.2	
2119	0.2	
2120	0.1	
2121	0.1	
2122	0.2	
2123	0.2	
2124	0.2	
2125	0.1	
2126	0.1	
2127	0.1	
2128	0.0	
2129	0.1	
2130	0.1	
2131	0.0	
2132	0.1	
2133	0.1	
2134	0.2	
2135	0.1	
2136	0.1	
2137	0.0	
2138	0.1	
2139		71.5
2140		81.4

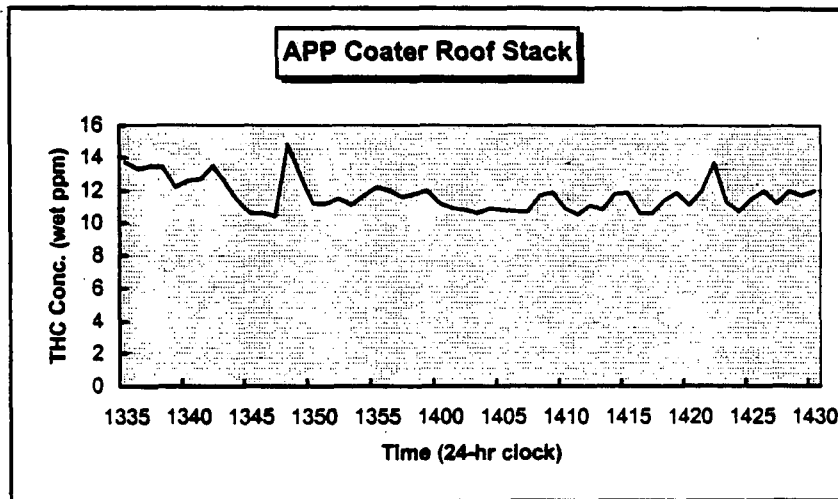
Run 3 Thermal Oxidizer Inlet/Outlet



U.S. Intec
Run 1 - APP Outlet Vent (T1)
Date: 9/24/97
Operator: Gulick

Time. (24 hr)	APP-T1 (ppm)
1335	13.7
1336	13.3
1337	13.5
1338	13.4
1339	12.2
1340	12.6
1341	12.7
1342	13.5
1343	12.5
1344	11.4
1345	10.6
1346	10.6
1347	10.4
1348	14.8
1349	12.9
1350	11.2
1351	11.2
1352	11.5
1353	11.1
1354	11.7
1355	12.2
1356	12.0
1357	11.6
1358	11.8
1359	12.0
1400	11.2
1401	10.9
1402	10.8
1403	10.6
1404	10.9
1405	10.8
1406	10.7
1407	10.7
1408	11.7
1409	11.9
1410	10.9
1411	10.5
1412	11.1
1413	10.8
1414	11.8

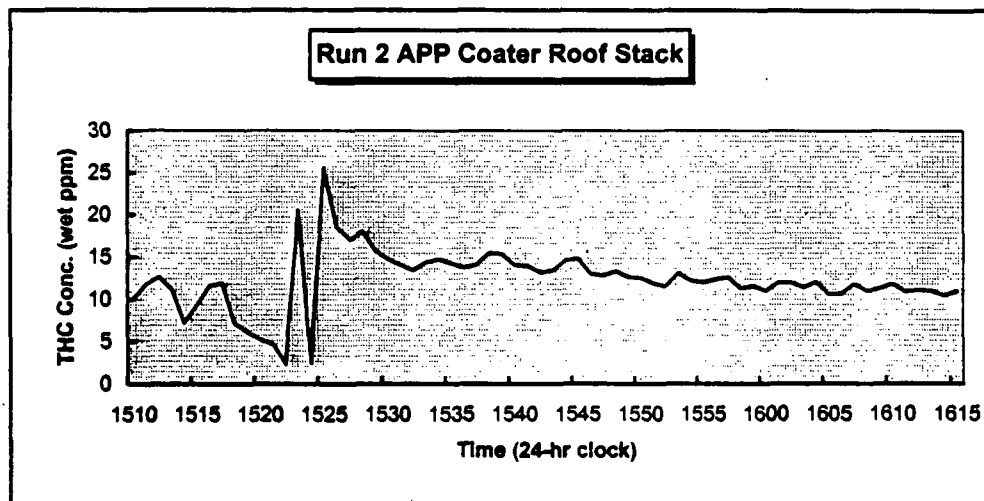
1415	11.9
1416	10.6
1417	10.6
1418	11.4
1419	11.9
1420	11.1
1421	12.0
1422	13.7
1423	11.3
1424	10.7
1425	11.5
1426	12.0
1427	11.2
1428	12.0
1429	11.7
1430	12.0



U.S. Intec
Run 2 - App Outlet Vent (T1)
Date: 9/24/97
Operator: Gulick

Time (24 hr)	APP-T1 (ppm)
1510	10.1
1511	11.8
1512	12.6
1513	11.1
1514	7.2
1515	9.3
1516	11.6
1517	11.9
1518	7.2
1519	6.1
1520	5.2
1521	4.7
1522	2.4
1523	20.5
1524	2.5
1525	25.5
1526	18.5
1527	17.0
1528	18.0
1529	15.7
1530	14.7
1531	14.0
1532	13.4
1533	14.4
1534	14.7
1535	14.2
1536	13.7
1537	14.1
1538	15.5
1539	15.3
1540	14.0
1541	13.9
1542	13.2
1543	13.4
1544	14.6
1545	14.8
1546	13.0
1547	12.8
1548	13.3
1549	12.6

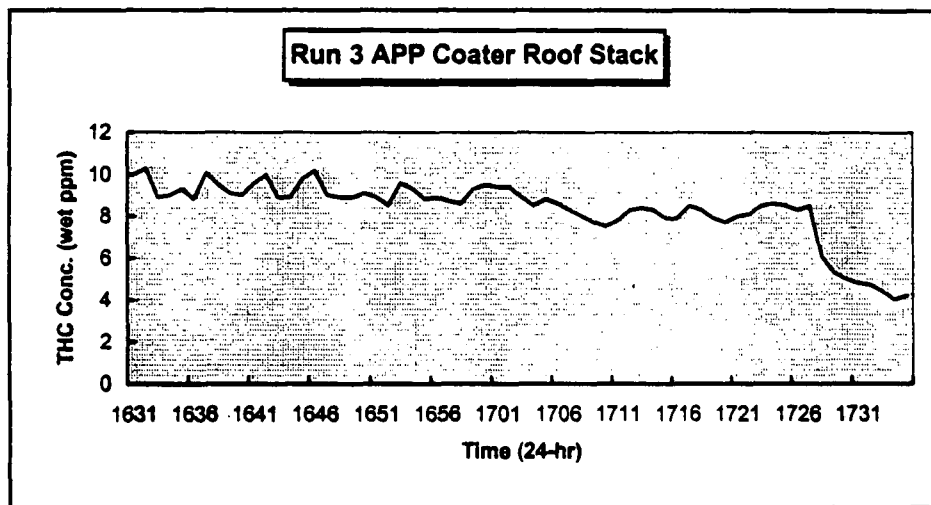
1550	12.5
1551	11.9
1552	11.5
1553	13.1
1554	12.2
1555	12.0
1556	12.4
1557	12.6
1558	11.3
1559	11.6
1600	11.0
1601	12.0
1602	12.0
1603	11.4
1604	12.1
1605	10.6
1606	10.7
1607	11.8
1608	11.0
1609	11.3
1610	11.8
1611	10.9
1612	11.1
1613	11.0
1614	10.4
1615	11.0



U.S. Intec
Run 3 - APP Outlet Vent (T1)
Date: 9/24/97
Operator: Gulick

Time (24 hr)	APP-T1 (ppm)
1631	10.0
1632	10.3
1633	8.9
1634	9.0
1635	9.3
1636	8.8
1637	10.1
1638	9.5
1639	9.1
1640	9.0
1641	9.6
1642	10.0
1643	8.9
1644	8.9
1645	9.8
1646	10.2
1647	9.0
1648	8.9
1649	8.9
1650	9.1
1651	8.9
1652	8.5
1653	9.6
1654	9.3
1655	8.8
1656	8.9
1657	8.7
1658	8.6
1659	9.3
1700	9.5
1701	9.4
1702	9.4
1703	8.9
1704	8.5
1705	8.8
1706	8.6
1707	8.3
1708	8.0
1709	7.7
1710	7.5

1711	7.8
1712	8.3
1713	8.4
1714	8.3
1715	7.9
1716	7.9
1717	8.5
1718	8.3
1719	7.9
1720	7.7
1721	8.0
1722	8.1
1723	8.5
1724	8.6
1725	8.5
1726	8.3
1727	8.5
1728	6.1
1729	5.3
1730	5.0
1731	4.8
1732	4.7
1733	4.4
1734	4.0
1735	4.2

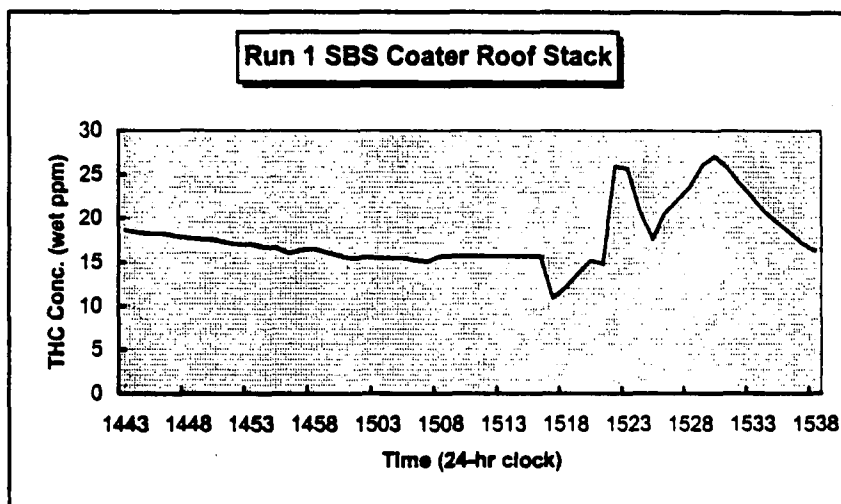


U.S. Intec
Run 1 - SBS Outlet Vent (T2)
Date: 9/24/97
Operator: Gulick

Time (24 hr)	SBS - T2 (ppm)
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1443	18.6
1444	18.3
1445	18.2
1446	18.2
1447	17.9
1448	17.7
1449	17.6
1450	17.5
1451	17.2
1452	17.0
1453	17.0
1454	16.7
1455	16.6
1456	16.0
1457	16.4
1458	16.5
1459	16.1
1500	15.7
1501	15.4
1502	15.6
1503	15.5
1504	15.5
1505	15.5
1506	15.2
1507	15.1
1508	15.7
1509	15.7
1510	15.7
1511	15.7
1512	15.7
1513	15.7
1514	15.7

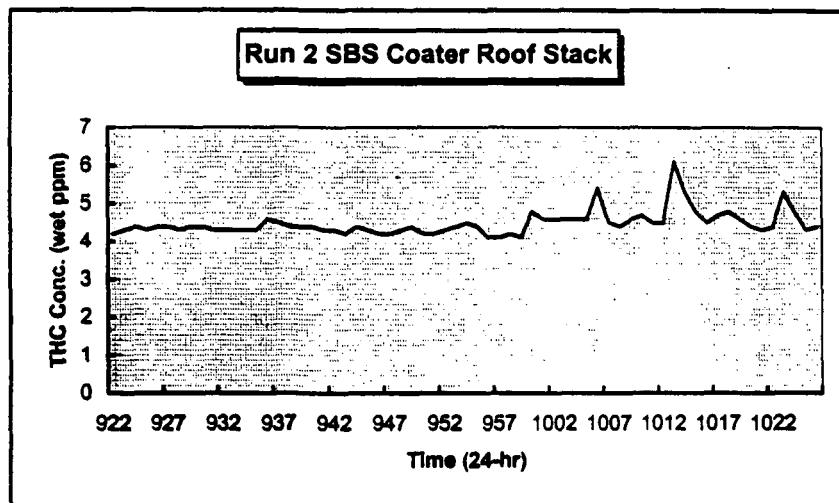
1515	15.7
1516	15.7
1517	10.9
1518	12.1
1519	13.7
1520	15.2
1521	14.8
1522	26.0
1523	25.7
1524	20.8
1525	17.6
1526	20.6
1527	22.1
1528	23.6
1529	26.1
1530	27.1
1531	25.8
1532	24.0
1533	22.4
1534	20.8
1535	19.5
1536	18.3
1537	17.1
1538	16.3



U.S. Intec
Run 2 - SBS Outlet Vent (T2)
Date: 9/25/97
Operator: Gulick

Time (24 hr)	SBS - T2 (ppm)
922	4.2
923	4.3
924	4.4
925	4.3
926	4.4
927	4.4
928	4.3
929	4.4
930	4.4
931	4.3
932	4.3
933	4.3
934	4.3
935	4.3
936	4.6
937	4.5
938	4.4
939	4.4
940	4.4
941	4.3
942	4.3
943	4.2
944	4.4
945	4.3
946	4.2
947	4.2
948	4.3
949	4.4
950	4.2
951	4.2
952	4.3
953	4.4
954	4.5
955	4.4
956	4.1
957	4.1
958	4.2
959	4.1
1000	4.8
1001	4.6

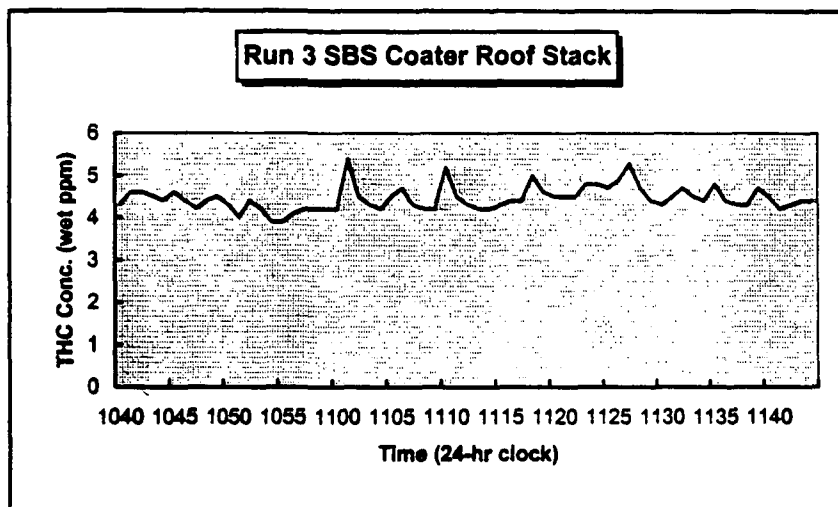
1002	4.6
1003	4.6
1004	4.6
1005	4.6
1006	5.4
1007	4.5
1008	4.4
1009	4.6
1010	4.7
1011	4.5
1012	4.5
1013	6.1
1014	5.3
1015	4.8
1016	4.5
1017	4.7
1018	4.8
1019	4.6
1020	4.4
1021	4.3
1022	4.4
1023	5.3
1024	4.8
1025	4.3
1026	4.4



U.S. Intec
Run 3 - SBS Outlet Vent (T2)
Date: 9/25/97
Operator: Gulick

Time (24 hr)	SBS - T2 (ppm)
1040	4.3
1041	4.6
1042	4.6
1043	4.5
1044	4.4
1045	4.6
1046	4.4
1047	4.2
1048	4.4
1049	4.5
1050	4.3
1051	4.0
1052	4.4
1053	4.2
1054	3.9
1055	3.9
1056	4.1
1057	4.2
1058	4.2
1059	4.2
1100	4.2
1101	5.4
1102	4.5
1103	4.3
1104	4.2
1105	4.5
1106	4.7
1107	4.3
1108	4.2
1109	4.2
1110	5.2
1111	4.5
1112	4.3
1113	4.2
1114	4.2
1115	4.3
1116	4.4
1117	4.4
1118	5.0
1119	4.6

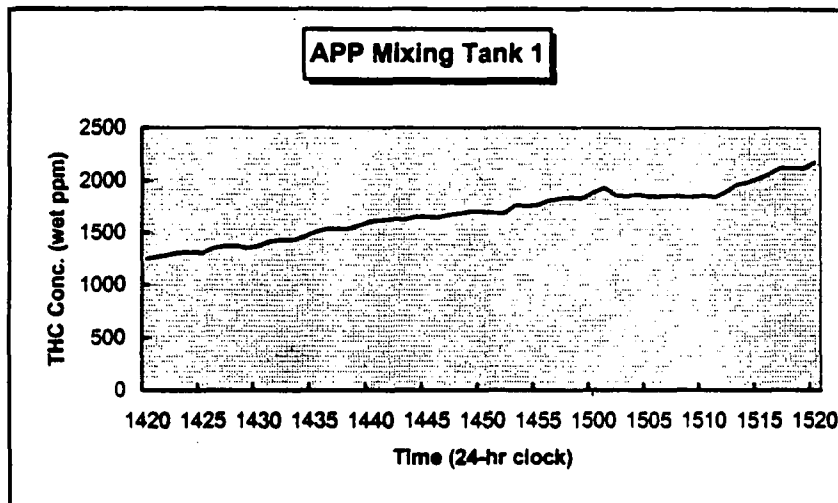
1120	4.5
1121	4.5
1122	4.5
1123	4.8
1124	4.8
1125	4.7
1126	4.9
1127	5.3
1128	4.7
1129	4.4
1130	4.3
1131	4.5
1132	4.7
1133	4.5
1134	4.4
1135	4.8
1136	4.4
1137	4.3
1138	4.3
1139	4.7
1140	4.5
1141	4.2
1142	4.3
1143	4.4
1144	4.4



U.S. Intec
Mixing Tank #1
Date: 9/25/97
Operator: Gulick

Time (24 hr)	Tank #1 THC (ppm)
1420	1253
1421	1270
1422	1290
1423	1309
1424	1312
1425	1307
1426	1351
1427	1368
1428	1370
1429	1352
1430	1372
1431	1413
1432	1430
1433	1425
1434	1453
1435	1503
1436	1531
1437	1536
1438	1534
1439	1567
1440	1606
1441	1616
1442	1630
1443	1621
1444	1654
1445	1649
1446	1644
1447	1671
1448	1683
1449	1706
1450	1702
1451	1687
1452	1688
1453	1763
1454	1756
1455	1766
1456	1809
1457	1828
1458	1837

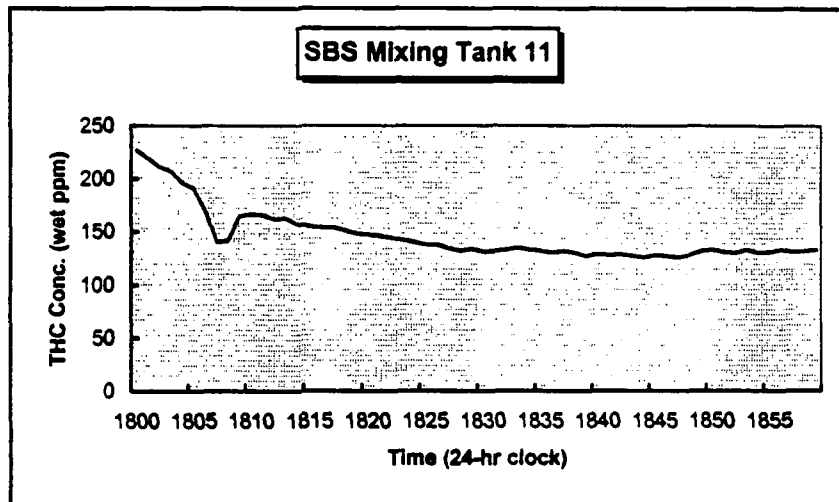
1459	1829
1500	1887
1501	1931
1502	1859
1503	1849
1504	1867
1505	1846
1506	1849
1507	1859
1508	1845
1509	1846
1510	1855
1511	1840
1512	1893
1513	1962
1514	1986
1515	2030
1516	2072
1517	2125
1518	2117
1519	2119
1520	2177



U.S. Intec
Mixing Tank #11
Date: 9/25/97
Operator: Gulick

Time (24 hr)	Tank #11 THC (ppm)
1800	227
1801	219
1802	211
1803	207
1804	196
1805	191
1806	170
1807	140
1808	142
1809	165
1810	167
1811	166
1812	162
1813	163
1814	157
1815	155
1816	154
1817	154
1818	151
1819	148
1820	147
1821	146
1822	144
1823	142
1824	140
1825	138
1826	138
1827	134
1828	132
1829	134
1830	131
1831	132
1832	133
1833	135
1834	133
1835	132
1836	130
1837	132
1838	130

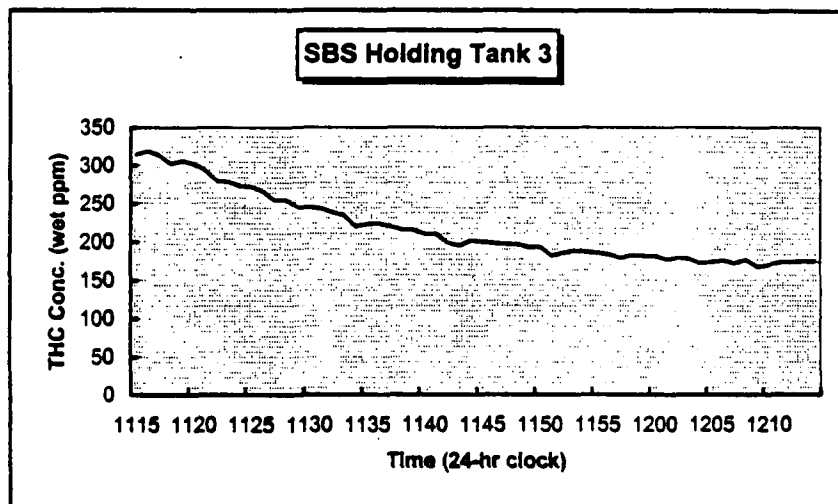
1839	127
1840	129
1841	128
1842	129
1843	127
1844	126
1845	128
1846	127
1847	126
1848	128
1849	132
1850	133
1851	131
1852	130
1853	133
1854	130
1855	131
1856	133
1857	131
1858	132
1859	133



U.S. Intec
SBS Holding Tank #3
Date: 9/26/97
Operator: Gulick

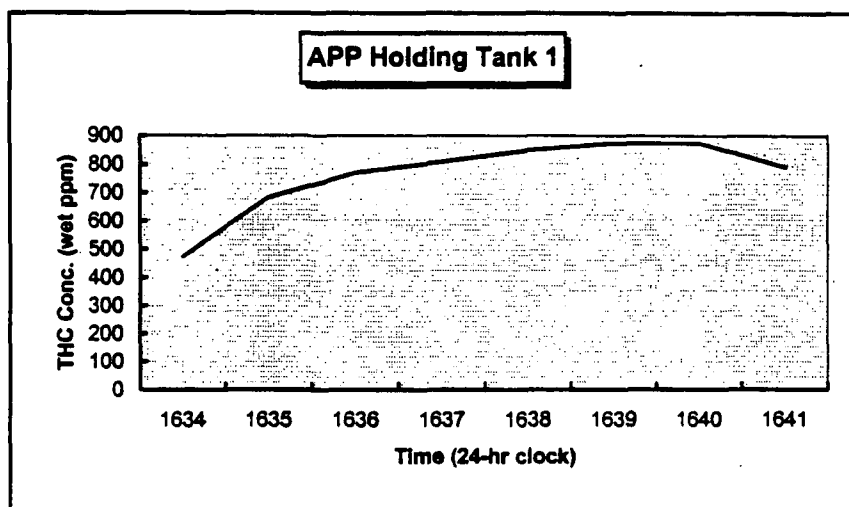
Time (24 hr)	Tank #3 THC (ppm)
1115	315
1116	319
1117	313
1118	302
1119	306
1120	302
1121	294
1122	280
1123	279
1124	273
1125	272
1126	266
1127	254
1128	255
1129	245
1130	245
1131	243
1132	238
1133	234
1134	220
1135	223
1136	224
1137	220
1138	216
1139	215
1140	210
1141	210
1142	199
1143	195
1144	202
1145	200
1146	198
1147	197
1148	197
1149	193
1150	194
1151	182
1152	186
1153	189

1154	187
1155	186
1156	184
1157	179
1158	183
1159	182
1200	182
1201	177
1202	179
1203	178
1204	172
1205	174
1206	176
1207	172
1208	177
1209	168
1210	170
1211	174
1212	174
1213	175
1214	175



U.S. Intec
APP Holding Tank #1
Date: 9/26/97
Operator: Gulick

Time (24 hr)	Tank #1 THC (ppm)
1634	473
1635	683
1636	771
1637	810
1638	849
1639	874
1640	874
1641	791



APPENDIX C
THC CALIBRATION RECORDS

Run 1 Thermal Oxidizer 9/22/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.0	0.0	Pass
	898.0		900.0	0.2	Pass
	502.0	503.1	500.0	0.6	Pass
	251.0	251.6	255.0	1.4	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	0.0	0.0	0.0	Pass

Instrument Span for THC 1 and 2 is 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	900.0	890.0	1.0	Pass

Instrument Span for THC 1 and 2 is 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Run 2 Thermal Oxidizer 9/23/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.8	0.1	Pass
	90.4		89.7	0.8	Pass
	50.3	50.3	49.9	0.7	Pass
	30.1	30.4	29.4	3.3	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	0.8	0.4	0.4	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	89.7	90.1	0.4	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	1
R Square	1
Adjusted R	65535
Standard Er	0
Observation	2

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>nificance F</i>
Regression	1	3952	3952	0	####
Residual	0	8E-28	65535		
Total	1	3952			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	0.8	0	65535	####	0.8	0.8	0.8	0.8
X Variable 1	0.9834071	0	65535	####	0.983	0.983	0.983	0.983

Run 3 Thermal Oxidizer 9/23/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.6	0.1	Pass
	90.4		90.1	0.3	Pass
	50.3	50.4	50.1	0.6	Pass
	30.1	30.4	30.1	1.0	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	0.6	0.7	0.1	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	90.1	90.0	0.1	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Run 1- SBS Outlet Vent 9/24/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.0	0.0	Pass
	90.4		90.9	0.6	Pass
	50.3	50.0	49.4	1.2	Pass
	30.1	29.9	29.1	2.8	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	0.0	0.1	0.1	Pass

Instrument Span for THC 1 is 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	90.9	90.3	0.6	Pass

Instrument Span for THC 1 is 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Runs 2 and 3 SBS Outlet Vent (T2) 9/24/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.2	0.0	Pass
	90.4		91.3	1.0	Pass
	50.3	50.9	49.4	2.9	Pass
	30.1	30.5	29.1	4.7	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	0.2	0.4	0.2	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	91.3	90.2	1.1	Pass

Instrument Span for THC 1 100 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	1
R Square	1
Adjusted R	65535
Standard Error	0
Observations	2

<i>ANOVA</i>					
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	4150	4150	0	#####
Residual	0	2E-28	65535		
Total	1	4150			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	0.2	0	65535	#####	0.2	0.2	0.2	0.2
X Variable 1	1.0077434	0	65535	#####	1.008	1.008	1.008	1.008

Mixing Tank # 1 9/25/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		4.8	0.0	Pass
	5003.0		4995.0	0.2	Pass
	2504.0	2502.4	2509.0	0.3	Pass
	1002.0	1004.2	1005.0	0.1	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	4.9	9.7	0.5	Pass

Instrument Span for THC 1 10000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	4990.0	5014.0	0.2	Pass

Instrument Span for THC 1 10000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

SUMMARY OUTPUT

Regression Statistics	
Multiple R	1
R Square	1
Adjusted R	65535
Standard Er	0
Observation	2

ANOVA

	df	SS	MS	F	Significance F
Regression	1	#####	#####	0	#####
Residual	0	2E-25	65535		
Total	1	#####			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.8	0	65535	#####	4.8	4.8	4.8	4.8
X Variable 1	0.9974415	0	65535	#####	0.997	0.997	0.997	0.997

Mixing Tank # 11 9/25/97

Calibration Error Determination

	Cal Gas Value	Predicted Value	Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		1.9	0.0	Pass
	898.0		899.0	0.1	Pass
	502.0	503.4	491.0	2.5	Pass
	251.0	252.6	255.0	0.9	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	1.9	0.5	0.1	Pass

Instrument Span for THC 1 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value	Final Value	Difference as % of Span	Pass/Fail
THC 1	899.0	896.0	0.3	Pass

Instrument Span for THC 1 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

SUMMARY OUTPUT

Regression Statistics	
Multiple R	1
R Square	1
Adjusted R	65535
Standard Error	0
Observations	2

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	#####	#####	0	#####
Residual	0	2E-26	65535		
Total	1	#####			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	1.9	0.65535	#####	1.9	1.9	1.9	1.9	1.9
X Variable 1	0.9989978	0.65535	#####	0.999	0.999	0.999	0.999	0.999

SBS Holding Tank # 3 9/26/97

Calibration Error Determination

	Cal Gas Value		Measured Value	Difference as % of Cal Gas	Pass/Fail
THC 1	0.0		0.0	0.0	Pass
	898.0		906.0	0.9	Pass
	502.0	506.5	496.0	2.1	Pass
	251.0	253.2	248.0	2.1	Pass

Pass/Fail Criteria is +/- 5% of Calibration Gas

Calibration Drift Determination

Zero Drift

	Initial Value		Final Value	Difference as % of Span	Pass/Fail
THC 1	0.0		0.5	0.1	Pass

Instrument Span for THC 1 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

Span Drift

	Initial Value		Final Value	Difference as % of Span	Pass/Fail
THC 1	906.0		904.0	0.2	Pass

Instrument Span for THC 1 1000 ppm

Pass/Fail Criteria is +/- 3% of Instrument Span

SUMMARY OUTPUT

Regression Statistics	
Multiple R	1
R Square	1
Adjusted R	65535
Standard Er	0
Observator	2

ANOVA

	df	SS	MS	F	Significance F
Regression	1	#####	#####	0	#####
Residual	0	1E-26	65535		
Total	1	#####			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	0	0	65535	#####	0	0	0	0
X Variable 1	1.0089087	0	65535	#####	1.009	1.009	1.009	1.009

APPENDIX D
FTIR FIELD DATA RECORDS

TABLE D-1. SUMMARY OF FTIR SPECTRAL FILES

Date	Time	Run No. & Location	Spectral Files	Notes
9/22	1450-1520	Run 1 T.O. Outlet	19220035-19220052	Computer error. Automated collection of files not working correctly.
	1520-1550	Run 1 T.O. Inlet	19220053-19220068	
	1550-1620	Run 1 T.O. Outlet	19220069-19220080	
	1620-1650	Run 1 T.O. Inlet	19220081-19220097	
	1650-1720	Run 1 T.O. Outlet	19220098-19220100	
	1720-1755	Run 1 T.O. Inlet	19220101-19220104	
	1755-1829	Run 1 T.O. Outlet	19220105-19220123	
	1829-1857	Run 1 T.O. Inlet	19220124-19220139	
	1857-1928	Run 1 T.O. Outlet	19220140-19220158	
9/23	1009-1045	Run 2 T.O. Outlet	19230006-19230024	Port change from 1230 to 1305.
	1045-1115	Run 2 T.O. Inlet	19230025-19230041	
	1115-1145	Run 2 T.O. Outlet	19230042-19230060	
	1145-1215	Run 2 T.O. Inlet	19230061-19230075	
	1215-1230	Run 2 T.O. Outlet	19230076-19230078	
	1305-1335	Run 2 T.O. Inlet	19230079-19230095	
	1335-1412	Run 2 T.O. Outlet	19230096-19230117	
	1412-1442	Run 2 T.O. Inlet	19230118-19230134	
	1442-1447	Run 2 T.O. Outlet	19230134-19230138	
9/23	1710-1740	Run 3 T.O. Inlet	19230140-19230157	Port change from 1918 to 1940.
	1740-1810	Run 3 T.O. Outlet	19230158-19230173	
	1810-1840	Run 3 T.O. Inlet	19230174-19230191	
	1840-1918	Run 3 T.O. Outlet	19230192-19230208	
	1940-2010	Run 3 T.O. Inlet	19230209-19230226	
	2010-2040	Run 3 T.O. Outlet	19230227-19230243	
	2040-2110	Run 3 T.O. Inlet	19230244-19230261	
	2110-2141	Run 3 T.O. Outlet	19230262-19230277	

TABLE D-1. SUMMARY OF FTIR SPECTRAL FILES (continued)

Date	Time	Run No. & Location	Spectral Files	Notes
9/24	1318-1437	Run 1, APP Coater Roof Stack	19240001-19240044	
	1437-1510	Run1, SBS Coater Roof Stack	19240045-19240063	
	1510-1610	Run 2, APP Coater Roof Stack	19240064-19240097	
	1610-1739	Run 3, APP Coater Roof Stack	19240098-19240147	
9/25	0921-1026	Run 2, SBS Coater Roof Stack	19250003-19250039	
	1040-1144	Run 3, SBS Coater Roof Stack	19250045-19250083	
	1404-1520	Run 1, APP Mixing Tank 1	19250097-19250139	
	1801-1902	Run 1, SBS Mixing Tank 11	19250146-19250178	
9/26	1115-1216	Run 1, SBS Holding Tank 3	19260007-19260040	
	1331-1431	Run 1, APP Holding Tank 1	19260043-19260075	Test repeated. Spectra were analyzed.
	1707-1808	Run 2, APP Holding Tank 1 (repeat test)	APP01-APP07	Computer error. Samples collected manually in batch mode. Samples APP03 and APP04 are dilutions of APP02.

FTIR FIELD DATA FORM

PROJECT NO. 3804-21

BAROMETRIC: _____

PLANT: Port Arthur

DATE: 9/22/97

OPERATOR: GmP/Suk

[illegible]

FTIR FIELD DATA FORM

BAROMETRIC:

DATE: 9/26/97

OPERATOR: S. Klammer

[illegible]

(Background and calibration spectra.)

BAROMETRIC:

OPERATOR: GMP/SK

[illegible]

(Background and calibration spectra.)

OPERATOR: Klamn

[illegible]

(Background and calibration spectra.)

PLANT: Port Arthur

DATE: 9/25/97

OPERATOR: Klammer

[illegible]

(Background and calibration spectra.)

BAROMETRIC:

OPERATOR: Klamn

[illegible]

FTIR FIELD DATA FORM
Sampling Data

PROJECT NO. 3304-21
 PLANT: PORT ARTHUR
 OPERATOR: KLamm

DATE: 9/22

BAROMETRIC: 29.98
 LEAK CHECK-START: _____
 LEAK CHECK-END: _____

SAMPLE TIME	FILE NAME	PATH	LOCATION / NOTES	NUMBER SCANS	RES (cm-1)	CELL TEMP (F)	SPIKED/ UNSPIKED	SAMPLE COND.	SAMPLE FLOW	CELL PRESS.	BKG
10:11			START AMBIENT CELL MONITOR	100	1.0	300	U	Amb	5 Cfm	770	B
10:53			MANUAL SPIKE TESTS / AMB (5.08 ppm SF6)								
11:29	SPSE001		Spike TOTAL FLOW = 6.0 CPM 2.0	100	1.0	300	S	Amb	6 LPM	780	B
11:34	SPSE002		Duplicate " " " "	100	1.0	300	S	Amb	6.0	780	B
11:39	SPTEL01		Toluene 60.6 ppm @ 2.0 LPM	100	1.0	300	S	Amb	6.0 LPM	780	B
11:43	SPTEL02		Dup. " " " "	100	1.0	300	S	Amb	6.0	780	B
11:53	DIRTEL01		TEL. Direct to cell 60.6 ppm	100	1.0	300	S	—	—	780	B
12:05	OUTUN01		outlet unspiked sample	100	1.0	300	U	STACK	6.0	780	B
12:11	OUTUN02		" " " "	100	1.0	300	U	STACK	6.0	780	B
12:20	OUTSP01		Spiked outlet w/ SF6 @ 2.0 LPM	100	1.0	300	S	STACK	6	780	B
12:25	OUTSP02		" " w/ TEL @ 60.6 ppm	100	1.0	300	S	STACK	6	780	B
12:35	INLUN01		Inlet unspiked sample	100	1.0	300	U	STACK	6	780	B
14:50	19220035		"SAMPLE 1" (outlet) - First one	100	1.0	300	U	STACK	5.5	780	B
			(start of test)								
15:20	19220053		" (Inlet) - Alternate location	100	1	300	U	STACK	6	780	B
15:50	19220069		(outlet)	100	1	300	U	"	6	780	B
16:20	19220081		(Inlet)	100	1	300	U	"	6	780	B
16:50	19220098		(outlet)	100	1	300	U	"	6	780	B
17:20			(Inlet) BATCH files not working								
17:48	19220101		Back on-line, (out of memory)	100	1	300	U	STACK	6	775	B
17:55	19220105		Switch to Outlet	100	1	300	U	"	"	"	B
18:27	19220124		Switch to Inlet ("Sample 2")	100	1	300	U	"	"	"	B
18:57	19220140		Switch to Outlet ("Sample 1")	100	1	300	U	"	"	"	B
19:56	DIR01		Direct to cell MFC #10.9 @ 2.0				S	Direct cell	5.0 ppm	765	B
			60.6 toluene 4.08 ppm SF6, 104 ppm p-Xylene								

Sampling Data

OPERATOR:

LEAK CHECK-END: _____

DATE: 9/22 (cont)

[illegible]

FTIR FIELD DATA FORM

Sampling Data

PROJECT NO. 3804-21
PLANT: Port Arthur
OPERATOR: Klamm

DATE: 9/23/97 (cont)

BAROMETRIC: 29.92
LEAK CHECK-START: —
LEAK CHECK-END: —

[illegible]

FTIR FIELD DATA FORM

Sampling Data

PROJECT NO. 3804-21
 PLANT: Port Arthur
 OPERATOR: S. Klammer

DATE: 9/25/97

BAROMETRIC: 29.93
 LEAK CHECK-START: —
 LEAK CHECK-END: —

SAMPLE TIME	FILE NAME	PATH	LOCATION / NOTES	NUMBER SCANS	RES (cm-1)	CELL TEMP (F)	SPIKED/ UNSPIKED	SAMPLE COND.	SAMPLE FLOW	CELL PRESS.	BKG
0918	19250001		N ₂ prior to test - possible bkgd.	100	1.0	240	U	N ₂ purge	6.0	770	A
0921	19250003		Switch to line 2 (SBS) - Test	100	1.0	240	U	STACK	6.0	775	A
1026	19250039		Continue monitoring - End Test.	100	1.0	240	U	STACK	6.0	775	A
1040	19250045		Start test. Continue monitoring	100	1.0	240	U	STACK	6.0	775	A
1144	19250083		End test. Stop monitoring.	100	1.0	240	U	STACK	6.0	775	A
1228	SB5SP01		Spike of SBS (line 2) post test	100	1.0	240	S	STACK	6.0	775	A
			MFC #2 @ 2.0 LPM (Sf ₆ + N ₂)								
1229	SB5SP02		Dup.								
1232	SB5SP03		Thp.								
1300	N201		N ₂ blank - stored in OTHERS	100	1.0	240	U	N ₂ purge	3.0	760	A
			very clean bkgd between test								
1305	19250089-96		On-line "monitor". Tank 1 App. (line 1)		1.0	240	U	Amplified STACK	6.0	770	A
1404	19250097		On-line in STACK Tank 1 App. (line 1)		1.0	240	U	STACK	6.0	770	A
1420	?		Start test. Incident w/THC.								
1520	19250139		End Test.								
	19250141		Purged. w/compounds 2900 d.		1.0	240	S	STACK	6.0	770	A
1549	F1SP01		Spike on line 1 MFC #2 @ 2.0 (Sf ₆ + N ₂)								
1551	19250142										
1553	19250143										
1558	PT01		Post test of Tank 1 - no dilution	100	1.0	240	U	STACK	6.0		
			(may contain some spike gas)								
1657	DIR05		Cal (spike) direct to cell	100	1.0	240	U	CAL	500 flow	760	A
1659	DIR06		Dup "								
1717	ETSP01		Ethylene Spike 2.0 LPM MFC #2								

FTIR FIELD DATA FORM

Sampling Data

PROJECT NO. 3504-21
 PLANT: Port Arthur
 OPERATOR: S. Klammer

DATE: 9/26/97

BAROMETRIC: _____
 LEAK CHECK-START: 58 mm Hg
 LEAK CHECK-END: _____

SAMPLE TIME	FILE NAME	PATH	LOCATION/NOTES	NUMBER SCANS	RES (cm-1)	CELL TEMP (F)	SPIKED/ UNSPIKED	SAMPLE COND.	SAMPLE FLOW	CELL PRESS.	BKG
1105	19260001	row 2	N ₂ blanks & start of test	100	1.0	240	N ₂ blank	—	6.0	770	A
1107	19260003		SBS Tank 3 (line 2)								
			Switch to Line 2 (SBS Tank 3)	100	1.0	240	STACK	of Ambient	6.0	770	A
1115	19260007		Tank closed - was ambient before	100	1.0	240	U	STACK	6.0	770	A
1216	19260040		STOP TEST	100	1.0	240	U	STACK	6.0	770	A
1240	T35P01		Spike Line 2 (SBS Tank 3)	100	1.0	240	S	STACK	6.0	770	A
			(Sf ₆ + xylene) MFC #2 & 2.0								
1245	T35P02										
1247	T35P03										
1329	19260041	19260042	N ₂ blanks prior to test	100	1.0	240	U	N ₂ purge	4.0	770	A
1331	19260043		START TEST APP Tank 1 (Line 1)	100	1.0	240	U	STACK	6.0	770	A
1419	19260069		Spike (TAC) w/ 6000 ppm propane								
1420	19260070		LK OK - sample no good								
1431	19260075		End Test								
1438	-0076		Restart Test								
1452	0083		End Test								
1505	0083 T35P04		Spike MFC #2 & 2.0 LPM	100	1.0	240	S	STACK	6.0	770	A
			(Sf ₆ + xylene) - NO GOOD								
1630/164	19260081	-85	N ₂ blanks prior to retest	100	1.0	240	U	NO N ₂	6.0	770	A
1645	19260086		Online SPS Tank 1 APP	100	1.0	240	U	STACK	4.0 (max)	760	A
1707	APP01		Manual collection Tank 1 APP	100	1.0	240	U	STACK	4.0	770	A
1716	APP02		" " " " " "	Appears							
1717	APP03		Dilution of APP02 (250 mm Hg)								
1724	APP04		Dilution of APP03 (second dilution)	to ~250							
1746	APP05		Manual collection	100	1.0	240	U	STACK	6.0	770	A

(FTIR Sampling Data)

BAROMETRIC: 29.98

DATE: 9/22/97

OPERATOR: Klammer

[illegible]

(FTIR Sampling Data)

BAROMETRIC: 29.92

OPERATOR: Klamn

[illegible]

(FTIR Sampling Data)

PLANT: Port Arthur

BAROMETRIC: 29.92

OPERATOR: Klamen

[illegible]

(FTIR Sampling Data)

BAROMETRIC: 29.85

OPERATOR: Klamath

[illegible]

FTIR FIELD DATA FORM

(FTIR Sampling Data)

PROJECT NO. 4701-08-05

BAROMETRIC: 29.93

PLANT: Port Arthur

DATE: 9/25/97

OPERATOR: Klam

SAMPLE TIME	FILE NAME	PATH		NUMBER SCANS	RES (cm-1)	CELL TEMP (F)	SPIKED/ UNSPIKED	SAMPLE COND.	SAMPLE FLOW	CELL PRESS	BKG
9:18	19250001		N2 prior to test - possible background	100	1	240	U	N2 purge	6	770	A
9:21	19250003		Switch to Line2(SBS) - test	100	1	240	U	STACK	6	775	A
10:26	19250039		Continue monitoring - end test	100	1	240	U	STACK	6	775	A
10:40	19250045		Start test - continue monitoring	100	1	240	U	STACK	6	775	A
11:44	19250083		End test - stop monitoring	100	1	240	U	STACK	6	775	A
12:26	SBSSP01		spike of SBS(Line2) post test	100	1	240	S	STACK	6	775	A
			MFC #2 @ 2.0 lpm (SF6 & xylene)								
12:29	SBSSP02		Dup. MFC #2 @ 2.0 lpm (SF6 & xylene)	100	1	240	S	STACK	6	775	A
12:32	SBSSP03		Trip. Dup MFC #2 @ 2.0 lpm (SF6 & xylene)	100	1	240	S	STACK	6	775	A
13:00	N201		N2 blank - stored in OTHERS	100	1	240	U	N2 purge	3	760	A
			very clean background between test								
13:05	19250089-96		On line "monitor" tank 1 app (Line1)	100	1	240	U	Ambient	6	770	A
14:04	19250097		On line "monitor" tank 1 app (Line1)	100	1	240	U	STACK	6	770	A
14:20			Start test coincident w/THC								
15:20	19250139		End test								
			Pegged with compound 2900d								
15:49	19250141		Spikes of line 1 MFC#2 @ 2.0 (SF6 & xylene)	100	1	240	S	STACK	6	770	A
15:51	19250142		Spikes of line 1 MFC#2 @ 2.0 (SF6 & xylene)	100	1	240	S	STACK	6	770	A
15:53	19250143		Spikes of line 1 MFC#2 @ 2.0 (SF6 & xylene)	100	1	240	S	STACK	6	770	A
15:58	PT01		Post test of tank 1 - no dilution	100	1	240	U	STACK	6		
			(may contain some spike gas)								
16:57	DIR05		Cal (spike) direct to cell	100	1	240	U	CAL	stop flow	760	A
16:59	DIR06		Dup Cal (spike) direct to cell								
17:19	ETSP01		Ethylene spike 2.0 lpm MFC #2								
17:58	19250144-145		Tank 11 - post test N2 blank	100	1	240	U	N2 blank	6	770	A
18:01	19250146		online "monitor" Tank 11 (Line 2)	100	1	240	U	STACK	6	770	A
19:02	19250		End test								
19:20	T11SP01		Spike MFC #2 @ 2.0 lpm (SF6 & xylene)	100	1	240	S	STACK	6	770	A
19:22	T11SP02		line 2 Spike MFC #2 @ 2.0 lpm (SF6 & xylene)	100	1	240	S	STACK	6	770	A
19:24	T11SP03		Spike MFC #2 @ 2.0 lpm (SF6 & xylene)	100	1	240	S	STACK	6	770	A
19:41	T1SP01		T1 spike (2nd try) w/SF6 + xylene MFC @ 2lpm	100	1	240	S	Ambient	6	770	A
19:44	T1SP02		T1 spike (2nd try) w/SF6 + xylene MFC @ 2lpm	100	1	240	S	Ambient	6	770	A
19:46	T1SP03		T1 spike (2nd try) w/SF6 + xylene MFC @ 2lpm	100	1	240	S	Ambient	6	770	A
20:04	PT02		Post test N2 blank - Background	100	1	240		N2 blank	6	770	A

(FTIR Sampling Date)

BAROMETRIC:

OPERATOR: Klamm

[illegible]

APPENDIX E
FTIR ANALYTICAL RESULTS

TABLE E-1. FTIR RESULTS AT THE THERMAL OXIDIZER INLET

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO		Formaldehyde	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/22/97 9/22/97 Run 1	11:39	INLUN01		0.080		0.369	6.786	0.419	3.574	0.438		0.537		0.343		0.058	2.818	0.383		3.697		0.545
	14:21	19220053		0.127		1.017		1.927		0.984	3.909	1.159		0.474		0.145		0.526		5.859		0.753
	14:23	19220054		0.097	3.591	0.416		1.612	6.063	0.582		0.774		0.396		0.084	2.578	0.441	12.971	4.223		0.630
	14:25	19220055	0.187	0.085	4.212	0.419		1.501	8.703	0.554		0.595		0.369		0.064	3.366	0.416	13.743	3.741		0.586
	14:27	19220056	0.186	0.081	1.582	0.411	5.235	0.487	8.558	0.502		0.552		0.361		0.060	3.722	0.400	13.823	3.599		0.574
	14:28	19220057	0.190	0.080	1.749	0.409	5.508	0.485	9.472	0.500		0.539		0.360		0.058	3.707	0.399	14.541	3.549		0.572
	14:30	19220058	0.228	0.081	2.279	0.418	5.754	0.495	11.543	0.511		0.547		0.369		0.059	4.063	0.407	16.163	3.600		0.586
	14:32	19220059	0.264	0.083	3.146	0.530		1.554	17.172	0.554		0.568	1.807	0.285		0.061	4.381	0.429	17.128	3.681		0.607
	14:34	19220060	0.241	0.083	2.805	0.529		1.543	16.306	0.552		0.562	1.815	0.284		0.061	4.116	0.427	16.428	3.656		0.603
	14:35	19220061	0.216	0.081	2.406	0.422	5.893	0.499	13.133	0.515		0.552		0.315		0.060	3.922	0.411	15.831	3.585		0.591
	14:37	19220062	0.191	0.080	2.209	0.417	5.864	0.493	12.263	0.509		0.545		0.311		0.059	3.713	0.406	15.170	3.536		0.583
	14:39	19220063	0.169	0.079	1.957	0.414	5.972	0.490	11.465	0.506		0.543		0.365		0.059	3.546	0.403	14.390	3.509		0.579
	14:41	19220064		0.080	1.804	0.414	6.037	0.491	10.883	0.506		0.541		0.364		0.058	3.411	0.403	12.660	3.485		0.578
	14:43	19220065		0.080	1.754	0.411	5.978	0.487	10.393	0.502		0.536		0.361		0.058	3.338	0.400	12.191	3.459		0.574
	14:44	19220066		0.080	1.730	0.411	5.988	0.487	10.076	0.502		0.533		0.361		0.058	3.296	0.400	11.803	3.463		0.573
	14:46	19220067		0.079	1.665	0.411	5.997	0.486	9.761	0.502		0.531		0.360		0.057	3.266	0.400	11.709	3.454		0.572
	14:48	19220068		0.078	1.673	0.407	5.949	0.483	9.559	0.498		0.518		0.357		0.056	3.256	0.397	11.679	3.411		0.567
	15:19	19220081		0.128		1.039		1.969		1.005	3.535	1.249		0.484		0.159		0.544		5.921		0.769
	15:21	19220082		0.121		0.999		1.892		0.966	3.810	1.192		0.465		0.149		0.523		5.619		0.739
	15:23	19220083		0.090	3.321	0.409		1.557	6.171	0.572		0.786		0.383		0.085	2.205	0.433	12.904	3.925		0.608
	15:24	19220084		0.076	4.431	0.366		1.396	9.103	0.512		0.563		0.343		0.061	3.010	0.388	13.035	3.292		0.545
	15:26	19220085		0.072	4.882	0.353		1.345	10.264	0.494		0.508		0.331		0.055	3.255	0.374	13.286	3.117		0.525
	15:28	19220086		0.069	4.661	0.372		1.330	10.842	0.491		0.492		0.327		0.053	3.368	0.370	13.582	3.055		0.519
	15:30	19220087		0.069	4.809	0.373		1.334	11.270	0.493		0.490		0.328		0.053	3.424	0.371	13.681	3.061		0.521
	15:31	19220088		0.071	4.872	0.376		1.343	11.430	0.497		0.488		0.330		0.053	3.459	0.374	13.868	3.095		0.525
	15:33	19220089		0.072	4.946	0.380		1.355	11.527	0.501		0.491		0.333		0.053	3.477	0.377	13.834	3.129		0.529
	15:35	19220090		0.072	5.033	0.383		1.364	11.602	0.505		0.493		0.335		0.053	3.474	0.380	13.706	3.150		0.533
	15:37	19220091		0.073	5.082	0.386		1.378	11.699	0.510		0.495		0.339		0.054	3.437	0.384	13.506	3.176		0.538
	15:38	19220092		0.074	5.093	0.389		1.386	11.643	0.513		0.501		0.341		0.054	3.425	0.386	13.285	3.198		0.541
	15:40	19220093		0.074	5.128	0.393		1.400	11.686	0.518		0.507		0.344		0.055	3.431	0.390	13.101	3.232		0.547
	15:42	19220094		0.075	5.185	0.398		1.418	11.754	0.525		0.513		0.349		0.055	3.432	0.395	12.875	3.262		0.554
	15:44	19220095		0.076	5.212	0.401		1.429	11.700	0.529		0.521		0.351		0.056	3.404	0.398	12.735	3.282		0.558
	15:45	19220096		0.076	5.267	0.404		1.443	11.759	0.534		0.524		0.355		0.057	3.387	0.402	13.138	3.322		0.564
	15:47	19220097		0.078	5.302	0.409		1.459	11.809	0.539		0.531		0.359		0.057	3.372	0.406	13.043	3.366		0.570
	16:47	19220101		0.077	4.144	0.586		1.466	13.742	0.544		0.530	1.100	0.288		0.057	3.082	0.406	10.847	3.309		0.572
	16:48	19220102		0.077	4.328	0.586		1.468	14.398	0.543		0.532	1.118	0.288		0.058	3.262	0.406	11.379	3.313		0.573
	16:50	19220103		0.077	4.472	0.589		1.480	15.499	0.546		0.537	1.157	0.289		0.058	3.283	0.408	11.535	3.328		0.578
	16:52	19220104		0.077	4.543	0.589		1.480	16.021	0.546		0.533	1.175	0.289		0.058	3.222	0.408	11.394	3.316		0.578
	17:27	19220124		0.128		1.078		2.042		1.043		1.474		0.502		0.159		0.564		5.932		0.798
	17:29	19220125		0.118		1.018		1.929	2.482	0.702		1.264		0.474		0.137		0.533		5.478		0.753
	17:31	19220126		0.089	4.818	0.428		1.624	9.326	0.599		0.735		0.399		0.079	2.570	0.454	12.155	3.874		0.634
	17:33	19220127		0.079	5.579	0.426		1.517	12.500	0.562		0.578		0.373		0.063	3.281	0.423	11.243	3.404		0.593
	17:34	19220128		0.075	4.379	0.589		1.468	13.910	0.547		0.533	1.099	0.289		0.058	3.288	0.409	10.680	3.228		0.573
	17:36	19220129		0.073	4.265	0.584		1.450	14.162	0.542		0.517	1.209	0.287		0.056	3.193	0.405	10.417	3.138		0.566
	17:38	19220130		0.072	4.229	0.583		1.444	14.208	0.541		0.506	1.244	0.286		0.055	3.073	0.404	10.150	3.101		0.564
	17:40	19220131		0.072	4.164	0.586		1.447	14.131	0.543		0.501	1.296	0.288		0.054	3.093	0.406	10.128	3.098		0.565
	17:41	19220132		0.072	4.171	0.588		1.452	14.142	0.546		0.501	1.345	0.289		0.054	3.103	0.408	9.964	3.119		0.567
	17:43	19220133		0.072	4.234	0.589		1.452	14.137	0.546		0.505	1.335	0.289		0.055	3.030	0.408	9.821	3.132		0.567
	17:45	19220134		0.073	4.508	0.593		1.466	14.314	0.550		0.508	1.303	0.291		0.055	3.550	0.411	10.741	3.167		0.573
	17:47	19220135		0.074	4.459	0.596		1.475	14.284	0.553		0.512	1.289	0.293		0.055	3.350	0.413	10.564	3.186		0.576
	17:49	19220136		0.074	4.321	0.596		1.475	14.065	0.553		0.517	1.293	0.293		0.056	3.077	0.413	10.142	3.197		0.576
	17:50	19220137		0.074	4.254	0.598		1.477	13.953	0.554		0.522	1.286	0.293		0.056	3.015	0.414	9.917	3.207		0.577
	17:52	19220138		0.074	4.238	0.598		1.477	13.923	0.555		0.523	1.277	0.294		0.057	3.031	0.415	9.965	3.221		0.577
	17:54	19220139		0.075	4.275	0.599		1.480	13.900	0.556		0.524	1.268	0.294		0.057	2.974	0.415	9.950	3.225		0.578
Average ---->			0.035	0.082	3.531	0.522	1.211	1.300	10.994	0.569	0.212	0.609	0.442	0.343		0.067	3.014	0.417	11.336	3.585		0.588

TABLE E-1. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO		Formaldehyde		
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	
9/23/97 Run 2	9:45	19230025		0.131		1.143		2.165		1.105		1.614		0.532		0.174		0.598		6.991		0.846	
	9:47	19230026		0.128		3.337	0.488	1.894		5.416	0.683	1.160		0.466		0.125		1.606	0.517	5.923		0.740	
	9:49	19230027		0.103		2.670	0.422	7.160	0.560	10.362	0.582	0.761		0.414		0.082		2.771	0.464	4.775		0.659	
	9:51	19230028		0.095		2.857	0.460	8.276	0.545	12.633	0.562	0.668		0.400		0.072		3.075	0.448	4.408		0.636	
	9:53	19230029		0.092		2.966	0.454	8.532	0.537	13.216	0.554	0.643		0.394	0.183	0.070		3.101	0.442	4.274		0.626	
	9:54	19230030		0.092		2.960	0.454	8.642	0.537	13.351	0.554	0.637		0.394			0.069		3.174	0.442	4.247		0.626
	9:56	19230031		0.092		2.959	0.456	8.789	0.540	13.384	0.557	0.641		0.396			0.069		3.284	0.444	4.279		0.629
	9:58	19230032		0.093		2.965	0.459	8.816	0.543	13.355	0.560	0.645		0.399			0.070		3.415	0.447	4.306		0.633
	10:00	19230033		0.093		3.020	0.462	8.851	0.547	13.394	0.564	0.651		0.402			0.070		3.577	0.450	4.323		0.638
	10:01	19230034		0.094		2.985	0.465	8.882	0.551	13.271	0.568	0.657		0.405			0.071		3.666	0.453	4.360		0.643
	10:03	19230035		0.094		2.780	0.464	8.880	0.549	12.806	0.567	0.656		0.403			0.071		3.624	0.452	4.339		0.640
	10:05	19230036		0.094		2.680	0.462	8.802	0.548	12.376	0.565	0.653		0.401			0.071		3.580	0.450	4.331		0.638
	10:07	19230037		0.092		2.565	0.458	8.628	0.543	12.199	0.560	0.644		0.398			0.070		3.427	0.446	4.277		0.632
	10:09	19230038		0.092		2.430	0.456	8.549	0.540	12.047	0.557	0.640		0.395			0.069		3.316	0.444	4.259		0.628
	10:10	19230039		0.092		2.441	0.458	8.661	0.543	12.208	0.560	0.641		0.397			0.069		3.413	0.446	4.279		0.631
	10:12	19230040		0.093		2.506	0.459	8.692	0.544	12.592	0.561	0.642		0.398			0.069		3.525	0.447	4.283		0.632
	10:14	19230041		0.093		2.444	0.458	8.689	0.543	12.685	0.560	0.639		0.397			0.069		3.225	0.446	4.281		0.630
	10:49	19230061		0.114		3.803	0.465		1.787	6.819	0.650	0.941		0.439			0.102		1.986	0.492	5.290		0.698
	10:51	19230062		0.096		5.275	0.419		1.589	10.573	0.586	0.687		0.391			0.074		2.854	0.444	4.435		0.620
	10:53	19230063		0.090		3.854	0.470	4.216	0.543	10.963	0.566	0.624		0.376			0.067		3.201	0.421	4.168		0.597
	10:55	19230064		0.088		3.838	0.462	4.514	0.534	11.274	0.557	0.604		0.369			0.065		3.180	0.414	4.069		0.587
	10:56	19230065		0.087		3.749	0.458	4.626	0.530	11.188	0.552	0.597		0.365			0.064		3.093	0.410	4.026		0.581
	10:58	19230066		0.087		3.720	0.460	4.762	0.532	11.185	0.554	0.598		0.366			0.065		3.061	0.412	4.040		0.582
	11:00	19230067		0.087		3.717	0.460	4.859	0.533	11.279	0.555	0.596		0.366			0.064		2.993	0.412	4.018		0.582
	11:02	19230068		0.087		3.512	0.463	4.930	0.536	10.866	0.558	0.598		0.368			0.065		2.991	0.415	4.034		0.585
	11:03	19230069		0.088		3.372	0.467	5.036	0.540	10.481	0.563	0.602		0.371			0.065		3.006	0.418	4.057		0.589
	11:05	19230070		0.089		3.384	0.471	5.204	0.545	10.381	0.568	0.610		0.374			0.066		3.014	0.422	4.100		0.594
	11:07	19230071		0.088		3.435	0.474	5.306	0.548	10.392	0.571	0.611		0.376			0.066		3.054	0.424	4.094		0.597
	11:09	19230072		0.089		3.423	0.476	5.359	0.550	10.413	0.574	0.611		0.378			0.066		3.125	0.426	4.114		0.600
	11:11	19230073		0.089		3.433	0.476	5.385	0.550	10.485	0.573	0.610		0.377			0.066		3.066	0.426	4.099		0.599
	11:12	19230074		0.089		3.465	0.475	5.453	0.550	10.660	0.573	0.609		0.377			0.066		3.074	0.426	4.102		0.599
	11:14	19230075		0.089		3.490	0.476	5.555	0.551	10.849	0.574	0.610		0.377			0.066		2.986	0.427	4.116		0.600
	12:05	19230079		0.084		3.727	0.452	3.832	0.523	11.068	0.545	0.574		0.357			0.062		3.647	0.405	3.870		0.568
	12:06	19230080		0.084		3.818	0.454	3.854	0.526	11.144	0.548	0.576		0.359			0.062		3.605	0.407	3.878		0.571
	12:08	19230081		0.084		3.917	0.457	3.921	0.529	11.392	0.551	0.582		0.362			0.063		3.525	0.410	3.891		0.575
12:10	19230082		0.085		3.890	0.461	4.022	0.533	11.479	0.555	0.590		0.365			0.064		3.473	0.413	3.921		0.579	
12:12	19230083		0.085		3.878	0.463	4.169	0.535	11.521	0.558	0.590		0.366			0.064		3.419	0.415	3.927		0.582	
12:13	19230084		0.085		3.856	0.464	4.225	0.536	11.528	0.559	0.590		0.367			0.064		3.378	0.415	3.922		0.583	
12:15	19230085		0.084		3.834	0.464	4.294	0.537	11.671	0.560	0.585		0.367			0.063		3.366	0.416	3.909		0.584	
12:17	19230086		0.084		3.763	0.464	4.428	0.536	11.753	0.559	0.582		0.366		0.063		3.313	0.415	3.902		0.582		
12:19	19230087		0.084		3.709	0.463	4.593	0.536	11.866	0.558	0.578		0.365		0.062		3.267	0.415	3.885		0.581		
12:21	19230088		0.084		3.735	0.464	4.781	0.536	12.047	0.559	0.576		0.366		0.062		3.257	0.415	3.887		0.581		
12:22	19230089		0.084		4.158	0.467	4.984	0.540	13.330	0.563	0.585		0.369		0.063		3.289	0.418	3.904		0.587		
12:24	19230090		0.085		3.930	0.468	5.117	0.542	13.216	0.565	0.586		0.370		0.063		3.222	0.420	3.921		0.588		
12:26	19230091		0.085		3.784	0.470	5.133	0.543	12.839	0.566	0.582		0.370		0.063		3.192	0.421	3.924		0.589		
12:28	19230092		0.084		3.750	0.470	5.121	0.544	12.724	0.567	0.583		0.371		0.063		3.182	0.421	3.864		0.589		
12:29	19230093		0.084		3.802	0.470	5.052	0.543	12.807	0.566	0.583		0.371		0.063		3.247	0.421	3.656	7.565	0.590		
12:31	19230094		0.084		3.924	0.471	5.084	0.545	13.239	0.568	0.586		0.373		0.063		3.244	0.422	3.663	7.510	0.592		
12:33	19230095		0.084		3.731	0.473	5.163	0.547	13.021	0.570	0.588		0.374		0.064		3.181	0.424	3.656		0.594		
13:14	19230118		0.112		3.943	0.475		1.796	7.455	0.665	0.945		0.442		0.102		1.804	0.504	5.200		0.702		
13:15	19230119		0.095		3.809	0.511	4.080	0.591	10.727	0.616	0.687		0.402		0.074		2.691	0.458	4.395		0.639		
13:17	19230120		0.090		3.999	0.497	4.843	0.575	11.684	0.599	0.628		0.390		0.068		2.831	0.445	4.148		0.619		
13:19	19230121		0.088		4.045	0.493	5.130	0.570	11.977	0.594	0.616		0.386		0.067		2.825	0.441	4.080		0.613		
13:21	19230122		0.088		3.986	0.489	5.193	0.566	11.996	0.590	0.605		0.383		0.065		2.789	0.438	4.053		0.609		
13:23	19230123		0.087		3.942	0.487	5.152	0.563	11.880	0.587	0.599		0.381		0.065								

TABLE E-1. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO		Formaldehyde	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
	13:37	19230131		0.088	3.691	0.489	4.212	0.566	10.804	0.590		0.604		0.382		0.065	2.722	0.438		4.087		0.608
	13:39	19230132		0.088	3.621	0.488	4.115	0.565	10.602	0.589		0.601		0.381		0.065	2.607	0.437		4.068		0.605
	13:40	19230133		0.088	3.525	0.488	4.095	0.564	10.402	0.588		0.598		0.380		0.065	2.562	0.437		4.061		0.604
	13:42	19230134		0.088	3.517	0.489	4.021	0.565	10.326	0.589		0.601		0.381		0.065	2.582	0.438		4.079		0.605
	13:49	19230138		0.103	4.489	0.453		1.688	8.899	0.634		0.745		0.415		0.081	2.070	0.480		4.761		0.659
	13:51	19230139		0.093	3.603	0.503	3.977	0.582	10.389	0.607		0.626		0.392		0.068	2.560	0.451		4.301		0.623
	14:12	INSP03		0.071	4.090	0.379		1.347	13.177	0.512	29.809	0.535		0.331	0.344	0.068	3.638	0.390	16.390	3.067		0.526
	14:14	INSP04		0.070	3.528	0.381		0.502	13.067	0.516	30.025	0.529		0.332	0.339	0.068	3.526	0.392	10.640	3.043		0.527
Average --->				0.091	3.508	0.480	5.136	0.661	11.284	0.584		0.648		0.387	0.003	0.070	2.995	0.438	0.222	4.206		0.614

TABLE E-1. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO		Formaldehyde		
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	
9/23/97 Run 3	16:10	19230140		0.075	3.629	0.411	6.177	0.551	11.532	0.507		0.493		0.350	0.144	0.053	4.429	0.394	6.564	3.254	3.209	0.536	
	16:11	19230141		0.082	3.753	0.448	6.602	0.570	12.520	0.537		0.539		0.383	0.159	0.057	4.767	0.423		3.816	3.421	0.587	
	16:13	19230142		0.085	3.663	0.459	6.916	0.584	12.531	0.550		0.553		0.392	0.164	0.059	4.748	0.434		3.930	3.456	0.601	
	16:15	19230143		0.086	3.621	0.463	7.024	0.589	12.336	0.555		0.556		0.396	0.161	0.059	4.795	0.437		3.965	3.435	0.607	
	16:17	19230144		0.087	3.618	0.469	7.187	0.596	12.477	0.562		0.563		0.400	0.163	0.060	4.611	0.442		4.009	3.460	0.614	
	16:18	19230145		0.087	3.603	0.471	7.288	0.600	12.520	0.565		0.565		0.402	0.165	0.060	4.507	0.445		4.031	3.475	0.617	
	16:20	19230146		0.088	3.671	0.473	7.282	0.602	12.513	0.567		0.568		0.404	0.166	0.060	4.585	0.447		4.057	3.551	0.620	
	16:22	19230147		0.088	3.793	0.477	7.274	0.607	12.731	0.572		0.574		0.407	0.167	0.061	4.737	0.450		3.821	3.634	0.625	
	16:24	19230148		0.089	4.003	0.478	7.093	0.608	13.009	0.573		0.581		0.408	0.175	0.062	4.958	0.451		3.845	3.684	0.626	
	16:25	19230149		0.089	4.371	0.479	6.691	0.610	13.622	0.574		0.585		0.409	0.177	0.062	5.304	0.452	8.619	3.878	3.682	0.628	
	16:27	19230150		0.090	4.464	0.483	6.926	0.649	13.809	0.596		0.589		0.412	0.180	0.062	5.272	0.464	8.651	3.897	3.719	0.630	
	16:29	19230151		0.090	4.348	0.484	6.867	0.650	13.892	0.598		0.591		0.413	0.186	0.063	5.186	0.465	8.507	3.900	3.696	0.632	
	16:31	19230152		0.090	4.237	0.483	6.955	0.649	13.776	0.596		0.589		0.411	0.178	0.062	5.186	0.464	8.131	3.898	3.641	0.630	
	16:33	19230153		0.090	4.359	0.484	6.902	0.649	13.865	0.597		0.589		0.412	0.179	0.062	5.489	0.464	8.349	3.915	3.605	0.631	
	16:34	19230154	0.196	0.091	4.716	0.494	6.843	0.664	14.260	0.610		0.604		0.421	0.183	0.064	5.774	0.474	9.926	4.031	3.585	0.645	
	16:36	19230155	0.196	0.091	4.784	0.495	6.772	0.665	14.407	0.611		0.604		0.422	0.183	0.064	5.810	0.475	10.821	4.037	3.609	0.646	
	16:38	19230156		0.091	4.584	0.491	6.841	0.659	14.328	0.606		0.592		0.418	0.176	0.063	5.653	0.471	9.700	3.961	3.575	0.641	
	16:40	19230157		0.090	4.587	0.491	6.971	0.660	14.409	0.606		0.588		0.418	0.175	0.062	5.628	0.471	9.500	3.929	3.698	0.641	
	17:10	19230174		0.142			1.105		2.093		1.068	3.763	1.340	0.515		0.168		0.578			6.576		0.817
	17:12	19230175		0.118	2.900	0.413			1.848	5.039	0.621		1.028	0.454	0.286	0.102	2.476	0.496		5.477		0.722	
	17:13	19230176		0.094	3.291	0.477	5.929	0.607	11.495	0.571		0.645		0.410	0.201	0.068	4.373	0.450	10.437	4.054	2.614	0.624	
	17:15	19230177		0.088	3.615	0.469	6.655	0.597	12.512	0.562		0.584		0.401	0.174	0.062	4.743	0.443	9.480	3.817	3.177	0.615	
	17:17	19230178		0.087	3.540	0.466	6.859	0.593	12.337	0.559		0.571		0.398	0.171	0.061	4.582	0.440	8.420	3.757	3.295	0.611	
	17:19	19230179		0.087	3.468	0.467	6.962	0.594	12.071	0.560		0.564		0.399	0.170	0.060	4.579	0.441	7.517	3.753	3.294	0.611	
	17:20	19230180		0.087	3.390	0.468	6.959	0.595	11.912	0.560		0.564		0.400	0.171	0.060	4.639	0.441		3.762	3.228	0.612	
	17:22	19230181		0.087	3.368	0.467	6.918	0.593	11.602	0.559		0.561		0.399	0.168	0.060	4.604	0.440		3.757	3.183	0.611	
	17:24	19230182		0.087	3.198	0.464	7.010	0.591	11.326	0.556		0.561		0.397	0.166	0.060	4.374	0.438	7.647	3.752	3.136	0.608	
	17:26	19230183		0.087	3.049	0.464	7.165	0.591	10.988	0.556		0.562		0.397	0.171	0.060	4.374	0.438	7.675	3.753	3.158	0.608	
	17:28	19230184		0.088	3.336	0.470	7.111	0.598	10.895	0.563		0.574		0.402	0.186	0.061	4.805	0.443	7.921	3.816	3.093	0.615	
	17:29	19230185		0.093	3.757	0.485	6.944	0.617	11.154	0.582		0.606		0.416	0.199	0.064	5.147	0.458	8.419	4.032	2.991	0.636	
	17:31	19230186		0.096	4.029	0.496	6.801	0.631	11.255	0.594		0.628		0.425	0.208	0.066	5.469	0.468	8.605	4.174	2.862	0.650	
	17:33	19230187		0.097	4.187	0.502	6.832	0.639	11.355	0.602		0.639		0.431	0.209	0.067	5.458	0.474	9.070	4.237	2.835	0.658	
	17:35	19230188		0.097	4.334	0.499	6.787	0.635	11.211	0.598		0.635		0.429	0.201	0.067	4.738	0.471	8.658	4.197	2.779	0.654	
	17:36	19230189		0.095	4.286	0.494	6.861	0.628	11.004	0.591		0.623		0.423	0.202	0.066	4.403	0.466		4.111	2.803	0.646	
	17:38	19230190		0.094	4.568	0.491	6.800	0.625	10.960	0.589		0.617		0.421	0.207	0.065	4.511	0.464		4.341	2.753	0.643	
	17:40	19230191		0.093	4.470	0.488	6.823	0.621	10.929	0.584		0.607		0.418	0.210	0.064	4.971	0.460		4.289	2.745	0.639	
	18:39	19230209		0.088	4.784	0.458	6.215	0.582	10.989	0.548		0.593		0.394	0.448	0.063	4.215	0.432	10.367	3.823	2.408	0.599	
	18:41	19230210		0.088	5.211	0.465	6.337	0.591	11.988	0.557		0.592		0.399	0.267	0.063	4.395	0.439	10.399	3.798	2.780	0.609	
	18:43	19230211		0.087	5.370	0.464	6.300	0.590	12.470	0.556		0.587		0.398	0.219	0.063	4.496	0.438	10.277	3.771	2.874	0.608	
	18:44	19230212		0.089	5.744	0.474	6.197	0.603	13.071	0.568		0.599		0.407	0.214	0.064	4.857	0.448	10.550	3.879	2.905	0.621	
	18:46	19230213		0.092	6.110	0.489	6.084	0.621	13.493	0.585		0.622		0.419	0.222	0.066	5.090	0.461	10.769	4.051	2.828	0.640	
	18:48	19230214		0.093	5.931	0.486	6.113	0.618	13.303	0.582		0.622		0.417	0.221	0.066	4.941	0.459	10.198	4.028	2.775	0.636	
	18:50	19230215		0.090	5.580	0.476	6.153	0.605	12.909	0.570		0.607		0.408	0.212	0.065	4.634	0.449	9.381	3.916	2.676	0.623	
	18:51	19230216		0.088	5.259	0.464	6.178	0.591	12.421	0.556		0.590		0.398	0.208	0.063	4.449	0.438	8.916	3.799	2.627	0.608	
	18:53	19230217		0.086	4.998	0.455	6.152	0.579	11.885	0.545		0.579		0.391	0.203	0.062	4.294	0.430	8.454	3.714	2.589	0.596	
	18:55	19230218		0.085	4.894	0.448	6.109	0.570	11.474	0.537		0.575		0.385	0.207	0.062	4.190	0.423	7.896	3.667	2.517	0.587	
18:57	19230219		0.084	4.833	0.446	6.107	0.567	11.198	0.534		0.572		0.383	0.208	0.061	4.068	0.421	7.634	3.637	2.484	0.584		
18:59	19230220		0.084	4.794	0.444	6.126	0.564	10.880	0.531		0.568		0.381	0.207	0.061	3.963	0.419		3.614	2.450	0.581		
19:00	19230221		0.083	4.624	0.441	6.152	0.561	10.634	0.528		0.565		0.379	0.205	0.061	3.878	0.416		3.835	2.365	0.577		
19:02	19230222		0.083	4.621	0.440	6.152	0.560	10.574	0.527		0.564		0.378	0.209	0.060	3.862	0.415		3.833	2.347	0.576		
19:04	19230223		0.083	4.612	0.441																		

TABLE E-1. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO		Formaldehyde	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
	19:55	19230252	0.079		4.181	0.420	5.738	0.539	11.200	0.501		0.543		0.362	0.202	0.059	4.046	0.399		3.668		0.576
	19:57	19230253	0.079		4.124	0.419	5.785	0.538	11.123	0.500		0.541		0.362	0.203	0.059	4.274	0.399		3.664		0.575
	19:59	19230254	0.079		3.932	0.416	5.821	0.534	10.956	0.496		0.543		0.359	0.206	0.059	3.968	0.396		3.655		0.571
	20:01	19230255	0.079		4.127	0.418	5.792	0.532	10.687	0.501		0.543		0.360	0.209	0.059	4.049	0.394		3.642	1.873	0.547
	20:02	19230256	0.079		4.203	0.419	5.828	0.533	10.739	0.502		0.542		0.360	0.210	0.059	4.099	0.395		3.643	1.863	0.548
	20:04	19230257	0.079		4.147	0.418	5.838	0.531	10.626	0.500		0.542		0.359	0.203	0.059	3.825	0.394		3.635	1.855	0.547
	20:06	19230258	0.079		4.027	0.417	5.875	0.530	10.558	0.499		0.539		0.359	0.202	0.059	3.662	0.393		3.639	1.883	0.546
	20:08	19230259	0.078		3.985	0.417	5.885	0.530	10.604	0.499		0.538		0.359	0.199	0.058	3.582	0.393		3.626	1.872	0.546
	20:09	19230260	0.078		3.730	0.415	5.889	0.533	10.945	0.496		0.534		0.359	0.199	0.058	3.451	0.395		3.618		0.570
	20:11	19230261	0.079		3.855	0.419	5.903	0.538	11.148	0.500		0.539		0.362	0.199	0.059	3.721	0.399		3.647		0.575
	21:00	19230265	0.062		3.975	0.380	3.675	0.451	10.303	0.475	28.074	0.465		0.318	0.365	0.057	3.532	0.374	10.708	2.664		0.505
	21:02	19230266	0.062		3.897	0.381	3.692	0.452	10.368	0.477	28.557	0.467		0.319	0.365	0.057	3.591	0.375	10.875	2.686		0.507
Average --->			0.005	0.088	4.166	0.466	6.150	0.642	11.449	0.560	0.052	0.600		0.396	0.194	0.064	4.361	0.437	4.221	3.920	2.328	0.610

TABLE E-2. FTIR RESULTS FROM THE THERMAL OXIDIZER OUTLET

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/22/97	11:10	OUTUN01	0.086		0.778		1.474		0.752		3.216	0.594	0.362		0.069		2.439	0.400		3.962
9/22/97	11:14	OUTUN02	0.116		0.937		1.774		0.906		3.879	0.986	0.436		0.125		1.493	0.478		5.359
9/22/97	11:25	OUTSP01	0.074		0.322		1.311		0.669		22.038	0.522	0.322	0.930	0.064		2.989	0.364	26.100	3.215
9/22/97	11:31	OUTSP02	0.072		0.679		1.286		0.657		3.821	0.535	0.316		0.064		2.773	0.358	11.664	3.130
9/22/97	13:50	19220035	0.137		1.063		2.014		1.028		3.649	1.263	0.495		0.161			0.556		6.354
9/22/97	13:51	19220036	0.141		1.092		2.069		1.056		3.735	1.296	0.509		0.165			0.572		6.503
9/22/97	13:53	19220037	0.141		1.099		2.082		1.063		3.848	1.307	0.512		0.166			0.575		6.524
9/22/97	13:55	19220038	0.140		1.092		2.070		1.056		3.877	1.306	0.509		0.166			0.572		6.470
9/22/97	13:57	19220039	0.140		1.095		2.075		1.059		3.826	1.311	0.510		0.167			0.573		6.473
9/22/97	13:58	19220040	0.139		1.091		2.067		1.055		3.930	1.312	0.508		0.167			0.571		6.439
9/22/97	14:00	19220041	0.139		1.092		2.069		1.056		3.933	1.310	0.509		0.167			0.572		6.436
9/22/97	14:02	19220042	0.139		1.094		2.073		1.058		3.903	1.309	0.510		0.167			0.573		6.452
9/22/97	14:04	19220043	0.139		1.087		2.059		1.051		3.837	1.301	0.506		0.166			0.569		6.419
9/22/97	14:05	19220044	0.138		1.078		2.041		1.042		3.772	1.294	0.502		0.165			0.564		6.366
9/22/97	14:07	19220045	0.137		1.066		2.019		1.031		3.669	1.284	0.496		0.163			0.558		6.329
9/22/97	14:09	19220046	0.136		1.060		2.008		1.025		3.669	1.280	0.493		0.163			0.555		6.293
9/22/97	14:11	19220047	0.135		1.058		2.005		1.023		3.626	1.275	0.493		0.162			0.554		6.245
9/22/97	14:13	19220048	0.135		1.058		2.004		1.023		3.690	1.283	0.493		0.163			0.554		6.238
9/22/97	14:14	19220049	0.134		1.057		2.002		1.022		3.736	1.283	0.492		0.163			0.553		6.214
9/22/97	14:16	19220050	0.134		1.061		2.010		1.026		3.745	1.288	0.494		0.164			0.555		6.220
9/22/97	14:18	19220051	0.135		1.064		2.015		1.028		3.759	1.289	0.495		0.164			0.557		6.229
9/22/97	14:20	19220052	0.135		1.066		2.019		1.031		3.811	1.291	0.496		0.164			0.558		6.225
9/22/97	14:50	19220069	0.078		0.408		0.484		0.499		0.506		0.358		0.055		3.344	0.398	11.737	3.371
9/22/97	15:00	19220070	0.133		1.073		2.033		1.038		4.291	1.288	0.500		0.161			0.562		6.162
9/22/97	15:01	19220071	0.133		1.074		2.035		1.039		3.798	1.280	0.500		0.163			0.562		6.145
9/22/97	15:03	19220072	0.132		1.073		2.033		1.038		3.784	1.275	0.500		0.162			0.562		6.116
9/22/97	15:05	19220073	0.133		1.076		2.038		1.040		3.758	1.278	0.501		0.162			0.563		6.132
9/22/97	15:07	19220074	0.134		1.082		2.050		1.047		3.808	1.278	0.504		0.162			0.566		6.180
9/22/97	15:08	19220075	0.134		1.079		2.044		1.043		3.671	1.274	0.503		0.162			0.565		6.184
9/22/97	15:10	19220076	0.133		1.075		2.037		1.040		3.676	1.269	0.501		0.161			0.563		6.172
9/22/97	15:12	19220077	0.133		1.072		2.032		1.037		3.655	1.266	0.499		0.161			0.561		6.157
9/22/97	15:14	19220078	0.133		1.074		2.034		1.038		3.620	1.264	0.500		0.161			0.562		6.148
9/22/97	15:15	19220079	0.133		1.079		2.043		1.043		3.624	1.265	0.502		0.161			0.564		6.165
9/22/97	15:17	19220080	0.132		1.070		2.027		1.035		3.582	1.262	0.498		0.160			0.560		6.104
9/22/97	15:49	19220098	0.078		0.412		1.473		11.770		0.544		0.531		0.057		3.369	0.409	12.654	3.407
9/22/97	15:51	19220099	0.084		0.405		1.545		10.205		0.566		0.583		0.063		3.024	0.429	12.926	3.662
9/22/97	15:52	19220100	0.114		0.976		1.849		4.847		0.669		1.082		0.117		1.390	0.522		5.266
9/22/97	16:54	19220105	0.076		0.586		1.468		15.532		0.543		0.526	1.198	0.057		3.132	0.406	11.303	3.268
9/22/97	16:56	19220106	0.077		0.592		1.484		14.599		0.549		0.533	1.104	0.058		3.005	0.411	11.415	3.320
9/22/97	16:57	19220107	0.103		0.461		1.745		6.340		0.645		0.956		0.103		1.508	0.488	9.476	4.689
9/22/97	16:59	19220108	0.119		1.013		1.919		2.453		0.697		1.289		0.139			0.530		5.526
9/22/97	17:01	19220109	0.125		1.047		1.984				1.013		1.397		0.151			0.548		5.790
9/22/97	17:03	19220110	0.127		1.063		2.014				1.028		1.440		0.156			0.557		5.885
9/22/97	17:04	19220111	0.128		1.071		2.029				1.036		1.456		0.157			0.561		5.930
9/22/97	17:06	19220112	0.129		1.076		2.038				1.040		1.466		0.158			0.563		5.950
9/22/97	17:08	19220113	0.130		1.086		2.058				1.050		1.482		0.160			0.569		5.996
9/22/97	17:10	19220114	0.129		1.085		2.056				1.049		1.477		0.160			0.568		5.980
9/22/97	17:11	19220115	0.129		1.083		2.052				1.047		3.953		0.159			0.567		5.958
9/22/97	17:13	19220116	0.128		1.081		2.048				1.045		3.961		0.159			0.566		5.929
9/22/97	17:15	19220117	0.128		1.081		2.048				1.045		3.931		0.158			0.566		5.926
9/22/97	17:17	19220118	0.128		1.080		2.046				1.044		3.974		0.158			0.565		5.930
9/22/97	17:19	19220119	0.128		1.079		2.043				1.043		3.888		0.158			0.565		5.931

TABLE E-2. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/22/97	17:20	19220120	0.128		1.075		2.037		1.040		1.455		0.501		0.157		0.563		5.930	
9/22/97	17:22	19220121	0.128		1.074		2.035		1.039		1.453		0.500		0.157		0.562		5.926	
9/22/97	17:24	19220122	0.128		1.075		2.036		1.039		1.450		0.500		0.157		0.562		5.921	
9/22/97	17:26	19220123	0.128		1.079		2.043		1.043		1.469		0.502		0.159		0.564		5.941	
9/22/97	17:56	19220140	0.075		4.208	0.601	1.483		13.891	0.557	0.523		1.275	0.295	0.057		2.925	0.417	9.900	3.227
9/22/97	17:57	19220141	0.077		6.133	0.405	1.516		12.474	0.566	0.543			0.373	0.059		2.852	0.429	10.202	3.345
9/22/97	17:59	19220142	0.105			0.953	1.806		6.244	0.667	0.997			0.444	0.108		1.334	0.520		4.877
9/22/97	18:01	19220143	0.121			1.043	1.976		2.149	0.722	1.300			0.486	0.141			0.546		5.608
9/22/97	18:03	19220144	0.126			1.076	2.037			1.040	1.399			0.501	0.151			0.563		5.846
9/22/97	18:04	19220145	0.128			1.088	2.061			1.052	1.434			0.507	0.155			0.569		5.932
9/22/97	18:06	19220146	0.129			1.096	2.076			1.060	1.451			0.510	0.157			0.574		5.979
9/22/97	18:08	19220147	0.130			1.100	2.084			1.064	1.466			0.512	0.158			0.576		5.995
9/22/97	18:10	19220148	0.129			1.098	2.079			1.061	1.461			0.511	0.158			0.574		5.972
9/22/97	18:11	19220149	0.129			1.099	2.082			1.063	1.464			0.512	0.158			0.575		5.970
9/22/97	18:13	19220150	0.129			1.097	2.079			1.061	4.015	1.268		0.511	0.159			0.574		5.952
9/22/97	18:15	19220151	0.129			1.097	2.078			1.061	4.002	1.270		0.511	0.159			0.574		5.949
9/22/97	18:17	19220152	0.129			1.098	2.079			1.061	4.008	1.269		0.511	0.159			0.575		5.959
9/22/97	18:18	19220153	0.129			1.098	2.080			1.062		1.465		0.511	0.158			0.575		5.953
9/22/97	18:20	19220154	0.129			1.096	2.076			1.060		1.462		0.510	0.158			0.574		5.949
9/22/97	18:22	19220155	0.128			1.094	2.073			1.058		1.455		0.509	0.157			0.573		5.944
9/22/97	18:24	19220156	0.128			1.092	2.069			1.056		1.449		0.509	0.157			0.572		5.944
9/22/97	18:25	19220157	0.128			1.089	2.064			1.053		1.450		0.507	0.157			0.570		5.941
9/22/97	18:27	19220158	0.128			1.089	2.063			1.053		1.452		0.507	0.157			0.570		5.939
9/22/97	19:08	OUTSP03	0.068			0.764	1.448			0.274	2.978	0.471		0.356	0.049		1.838	0.439		3.156
9/22/97	19:11	OUTSP04	0.070			0.784	1.485			0.289		0.469		0.365	0.051		1.716	0.464		3.243
Average --->			0.125		0.484	1.008	0.085	1.965	1.549	0.970	1.986	1.250	0.050	0.483		0.148	0.365	0.547	1.262	5.772

TABLE E-2. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/23/97	9:12	19230006		0.113		0.863		1.634		0.834		1.192		0.402	0.621	0.115		0.451	11.075	5.169
9/23/97	9:14	19230007		0.142		1.054		1.997		1.019		1.526		0.491		0.165		0.552		6.550
9/23/97	9:15	19230008		0.145		1.086		2.057		1.050		1.565		0.506		0.169		0.568		6.732
9/23/97	9:17	19230009		0.146		1.096		2.075		1.059		1.584		0.510		0.171		0.573		6.765
9/23/97	9:19	19230010		0.148		1.110		2.104		1.074		1.597		0.517		0.173		0.581		6.829
9/23/97	9:21	19230011		0.148		1.113		2.109		1.077		1.605		0.518		0.173		0.583		6.834
9/23/97	9:22	19230012		0.148		1.117		2.116		1.080		1.608		0.520		0.174		0.584		6.854
9/23/97	9:24	19230013		0.148		1.118		2.118		1.081		1.607		0.521		0.174		0.585		6.869
9/23/97	9:26	19230014		0.148		1.114		2.110		1.077		1.598		0.519		0.173		0.583		6.855
9/23/97	9:28	19230015		0.147		1.109		2.101		1.072		1.588		0.516		0.172		0.580		6.817
9/23/97	9:30	19230016		0.147		1.105		2.094		1.069		1.585		0.515		0.171		0.578		6.811
9/23/97	9:31	19230017		0.148		1.111		2.104		1.074		1.589		0.517		0.172		0.581		6.869
9/23/97	9:33	19230018		0.149		1.115		2.113		1.079		1.590		0.519		0.172		0.584		6.905
9/23/97	9:35	19230019		0.148		1.111		2.104		1.074		1.588		0.517		0.172		0.581		6.863
9/23/97	9:37	19230020		0.149		1.119		2.121		1.082		1.604		0.521		0.173		0.586		6.903
9/23/97	9:38	19230021		0.149		1.128		2.137		1.091		1.602		0.525		0.173		0.590		6.918
9/23/97	9:40	19230022		0.150		1.134		2.148		1.097		1.610		0.528		0.174		0.593		6.943
9/23/97	9:42	19230023		0.149		1.131		2.143		1.094		1.609		0.527		0.174		0.592		6.903
9/23/97	9:44	19230024		0.150		1.138		2.156		1.101		1.614		0.530		0.174		0.596		6.951
9/23/97	10:16	19230042		0.114	4.742	0.461		1.754	8.697	0.645		0.899		0.431		0.097	2.075	0.488		5.270
9/23/97	10:17	19230043		0.139		1.061		2.009	3.007	0.709		1.410		0.494		0.152		0.554		6.432
9/23/97	10:19	19230044		0.145		1.106		2.095		1.070		1.537		0.515		0.166		0.579		6.722
9/23/97	10:21	19230045		0.146		1.120		2.121		1.083		1.567		0.521		0.169		0.586		6.759
9/23/97	10:23	19230046		0.146		1.123		2.127		1.086		1.581		0.523		0.171		0.588		6.755
9/23/97	10:25	19230047		0.146		1.127		2.134		1.089		1.582		0.525		0.171		0.590		6.761
9/23/97	10:26	19230048		0.147		1.129		2.140		1.092		1.582		0.526		0.171		0.591		6.784
9/23/97	10:28	19230049		0.147		1.132		2.144		1.094		1.588		0.527		0.172		0.592		6.810
9/23/97	10:30	19230050		0.147		1.124		2.129		1.087		1.579		0.523		0.171		0.588		6.783
9/23/97	10:32	19230051		0.145		1.112		2.107		1.076		1.570		0.518		0.170		0.582		6.730
9/23/97	10:33	19230052		0.145		1.110		2.103		1.073		1.560		0.517		0.169		0.581		6.725
9/23/97	10:35	19230053		0.145		1.105		2.093		1.069		1.555		0.515		0.168		0.578		6.707
9/23/97	10:37	19230054		0.145		1.105		2.093		1.068		1.560		0.514		0.169		0.578		6.695
9/23/97	10:39	19230055		0.148		1.129		2.139		1.092		1.578		0.526		0.171		0.591		6.855
9/23/97	10:40	19230056		0.151		1.153		2.184		1.115		1.597		0.537		0.173		0.603		6.990
9/23/97	10:42	19230057		0.151		1.154		2.187		1.116		1.602		0.538		0.173		0.604		6.973
9/23/97	10:44	19230058		0.150		1.154		2.187		1.116		1.601		0.538		0.173		0.604		6.943
9/23/97	10:46	19230059		0.154		1.184		2.243		1.145		1.626		0.551		0.176		0.620		7.109
9/23/97	10:48	19230060		0.152		1.180		2.235		1.141		1.589		0.549		0.172		0.618		7.047
9/23/97	11:16	19230076		0.113	3.875	0.460		1.749	6.890	0.643		0.903		0.430		0.098	1.855	0.487		5.208
9/23/97	11:18	19230077		0.138		1.069		2.024	2.430	0.720		1.393		0.498		0.151		0.559		6.366
9/23/97	11:19	19230078		0.138		1.083		2.052		1.048		1.351		0.504		0.146		0.567		6.406
9/23/97	11:50	OUTSP05		0.086		0.437		1.554		0.306	24.271	0.620		0.382	0.416	0.076	2.593	0.446	11.275	3.707
9/23/97	11:52	OUTSP06		0.085		0.436		1.548		0.305	24.537	0.617		0.381	0.412	0.076	2.587	0.445	11.293	3.691
9/23/97	12:35	19230096		0.084	3.652	0.473	5.213	0.547	12.903	0.570		0.586		0.373		0.063	3.090	0.424		3.658
9/23/97	12:37	19230097		0.108	3.810	0.458		1.734	8.009	0.640		0.878		0.426		0.095	1.926	0.485		4.995
9/23/97	12:38	19230098		0.134		1.067		2.021	2.774	0.725		1.381		0.497		0.149		0.558		6.205
9/23/97	12:40	19230099		0.142		1.113		2.109		1.076		1.512		0.518		0.163		0.583		6.558
9/23/97	12:42	19230100		0.144		1.126		2.134		1.089		1.559		0.524		0.169		0.589		6.673
9/23/97	12:44	19230101		0.144		1.128		2.137		1.091		1.554		0.525		0.168		0.590		6.681
9/23/97	12:45	19230102		0.145		1.131		2.142		1.094		1.561		0.527		0.169		0.592		6.697
9/23/97	12:47	19230103		0.145		1.135		2.150		1.097		1.568		0.528		0.169		0.594		6.717

TABLE E-2. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/23/97	12:49	19230104	0.146		1.142		2.163		1.104		1.570		0.532		0.170		0.598		6.748	
9/23/97	12:51	19230105	0.146		1.150		2.178		1.112		1.582		0.535		0.171		0.602		6.756	
9/23/97	12:52	19230106	0.146		1.154		2.185		1.115		1.584		0.537		0.171		0.604		6.761	
9/23/97	12:54	19230107	0.146		1.157		2.193		1.119		1.588		0.539		0.172		0.606		6.776	
9/23/97	12:56	19230108	0.147		1.158		2.194		1.120		1.589		0.539		0.172		0.606		6.779	
9/23/97	12:58	19230109	0.146		1.152		2.182		1.114		1.587		0.536		0.172		0.603		6.776	
9/23/97	13:00	19230110	0.146		1.149		2.178		1.112		1.586		0.535		0.171		0.602		6.767	
9/23/97	13:01	19230111	0.146		1.147		2.174		1.110		1.585		0.534		0.171		0.601		6.769	
9/23/97	13:03	19230112	0.146		1.144		2.168		1.107		1.572		0.533		0.170		0.599		6.760	
9/23/97	13:05	19230113	0.146		1.143		2.164		1.105		1.566		0.532		0.169		0.598		6.756	
9/23/97	13:07	19230114	0.146		1.142		2.163		1.104		1.568		0.532		0.170		0.598		6.758	
9/23/97	13:08	19230115	0.146		1.144		2.167		1.106		1.569		0.533		0.170		0.599		6.749	
9/23/97	13:10	19230116	0.146		1.149		2.177		1.111		1.573		0.535		0.170		0.601		6.765	
9/23/97	13:12	19230117	0.144		1.138		2.155		1.100		1.544		0.530		0.167		0.595		6.657	
9/23/97	13:44	19230135	0.118		0.978		1.852	6.308	0.681		1.015		0.455		0.110	1.350	0.531		5.463	
9/23/97	13:46	19230136	0.139		1.100		2.084	2.103	0.754		1.431		0.512		0.155		0.576		6.420	
9/23/97	13:47	19230137	0.133		1.065		2.017	3.243	0.731		1.294		0.496		0.140		0.557		6.164	
Average ---->			0.143		0.244	1.077	0.079	2.075	0.854	1.025	1.501		0.514		0.009	0.162	0.156	0.578	0.168	6.591

TABLE E-2. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/23/97	16:41	19230158	0.113		4.308	0.410		1.818	7.698	0.617		0.886	0.447		0.266	0.089	3.533	0.493	12.208	4.924
9/23/97	16:43	19230159	0.137		2.306	0.495		2.026		1.034	3.835	1.209	0.498			0.151	1.716	0.538		6.328
9/23/97	16:45	19230160	0.141			1.096		2.076		1.060	3.691	1.294	0.510			0.162	1.395	0.552		6.522
9/23/97	16:47	19230161	0.142			1.106		2.096		1.070	3.801	1.325	0.515			0.166		0.579		6.578
9/23/97	16:49	19230162	0.142			1.108		2.099		1.071	3.770	1.332	0.516			0.167		0.580		6.594
9/23/97	16:50	19230163	0.143			1.112		2.107		1.075	3.785	1.346	0.518			0.169		0.582		6.623
9/23/97	16:52	19230164	0.143			1.109		2.101		1.072	3.737	1.338	0.516			0.168		0.580		6.599
9/23/97	16:54	19230165	0.143			1.108		2.098		1.071	3.760	1.339	0.516			0.168		0.580		6.602
9/23/97	16:56	19230166	0.143			1.106		2.095		1.069	3.729	1.335	0.515			0.167		0.579		6.608
9/23/97	16:57	19230167	0.143			1.105		2.094		1.069	3.706	1.332	0.515			0.167		0.579		6.610
9/23/97	16:59	19230168	0.143			1.104		2.092		1.068	3.616	1.326	0.514			0.166		0.578		6.597
9/23/97	17:01	19230169	0.143			1.105		2.092		1.068	3.635	1.326	0.514			0.166		0.578		6.602
9/23/97	17:03	19230170	0.143			1.106		2.095		1.069	3.623	1.329	0.515			0.166		0.579		6.617
9/23/97	17:04	19230171	0.143			1.104		2.091		1.067	3.609	1.328	0.514			0.166		0.578		6.607
9/23/97	17:06	19230172	0.142			1.102		2.088		1.066	3.687	1.333	0.513			0.167		0.577		6.590
9/23/97	17:08	19230173	0.142			1.101		2.085		1.064	3.714	1.334	0.513			0.167		0.576		6.566
9/23/97	17:42	19230192	0.114		2.516	0.469	4.057	0.657	5.132	0.610		0.899	0.449		0.271	0.090	3.096	0.488		5.295
9/23/97	17:43	19230193	0.138		2.162	0.502		2.051		1.047	3.797	1.217	0.504			0.152	1.597	0.545		6.390
9/23/97	17:45	19230194	0.143			1.113		2.108		1.076	3.638	1.309	0.518			0.164	1.230	0.563		6.640
9/23/97	17:47	19230195	0.144			1.115		2.112		1.078	3.666	1.329	0.519			0.166		0.584		6.660
9/23/97	17:49	19230196	0.144			1.116		2.114		1.079	3.651	1.336	0.520			0.167		0.584		6.662
9/23/97	17:51	19230197	0.146			1.132		2.144		1.095	3.667	1.359	0.527			0.170		0.592		6.765
9/23/97	17:52	19230198	0.151			1.169		2.215		1.131	3.913	1.380	0.544			0.173		0.612		6.971
9/23/97	17:54	19230199	0.150			1.165		2.206		1.126	3.948	1.375	0.542			0.172		0.610		6.929
9/23/97	17:56	19230200	0.147			1.148		2.174		1.110	3.927	1.364	0.534			0.171		0.601		6.822
9/23/97	17:58	19230201	0.146			1.137		2.154		1.099	3.800	1.357	0.529			0.170		0.595		6.767
9/23/97	17:59	19230202	0.145			1.130		2.140		1.092	3.722	1.347	0.526			0.169		0.591		6.723
9/23/97	18:01	19230203	0.145			1.123		2.128		1.086	3.684	1.341	0.523			0.168		0.588		6.710
9/23/97	18:03	19230204	0.145			1.119		2.121		1.082	3.623	1.337	0.521			0.167		0.586		6.688
9/23/97	18:05	19230205	0.144			1.117		2.117		1.081	3.604	1.336	0.520			0.167		0.585		6.678
9/23/97	18:07	19230206	0.144			1.115		2.112		1.078	3.617	1.336	0.519			0.167		0.583		6.660
9/23/97	18:08	19230207	0.144			1.117		2.116		1.080	3.642	1.338	0.520			0.168		0.584		6.674
9/23/97	18:10	19230208	0.144			1.117		2.115		1.080	3.698	1.341	0.520			0.168		0.584		6.662
9/23/97	18:19	OUTSP07	0.088		0.813		1.541		0.786		3.244	0.551	0.379		3.347	0.068	3.075	0.413	45.809	3.801
9/23/97	18:21	OUTSP08	0.084		0.802		1.519		0.775		2.676	0.537	0.373		3.572	0.061	2.932	0.407	16.773	3.639
9/23/97	18:34	OUTSP09	0.083		0.789		1.496		0.763			0.565	0.368		3.559	0.061	2.863	0.402	11.095	3.572
9/23/97	19:11	19230227	0.101		3.219	0.431	4.276	0.604	6.603	0.561		0.785	0.411		0.254	0.080	2.907	0.448		4.696
9/23/97	19:13	19230228	0.126		2.854	0.462		1.878		0.959		1.274	0.462			0.138	1.536	0.501		5.813
9/23/97	19:15	19230229	0.134			1.040		1.969		1.005	3.761	1.252	0.484			0.156	1.248	0.526		6.202
9/23/97	19:16	19230230	0.137			1.058		2.005		1.023	3.541	1.301	0.493			0.163	1.134	0.535		6.344
9/23/97	19:18	19230231	0.138			1.066		2.019		1.030	3.621	1.316	0.496			0.165		0.558		6.375
9/23/97	19:20	19230232	0.138			1.066		2.020		1.031	3.619	1.325	0.497			0.166		0.558		6.375
9/23/97	19:22	19230233	0.137			1.062		2.012		1.027	3.648	1.321	0.494			0.165		0.556		6.328
9/23/97	19:23	19230234	0.136			1.056		2.001		1.021	3.593	1.316	0.492			0.165		0.553		6.308
9/23/97	19:25	19230235	0.136			1.052		1.993		1.017	3.567	1.311	0.490			0.164		0.550		6.292
9/23/97	19:27	19230236	0.136			1.050		1.990		1.016	3.495	1.311	0.489			0.164		0.550		6.307
9/23/97	19:29	19230237	0.136			1.051		1.990		1.016		1.509	0.489			0.163		0.550		6.311
9/23/97	19:30	19230238	0.136			1.049		1.986		1.014		1.506	0.488			0.163		0.549		6.308
9/23/97	19:32	19230239	0.137			1.050		1.990		1.016		1.509	0.489			0.163		0.550		6.318
9/23/97	19:34	19230240	0.136			1.048		1.985		1.013	3.387	1.301	0.488			0.163		0.548		6.299
9/23/97	19:36	19230241	0.136			1.043		1.976		1.009	3.415	1.303	0.486			0.163		0.546		6.274

TABLE E-2. (continued)

Date	Time	File name	Carbonyl sulfide		Propane		Cumene		Hexane		p-Xylene		2,2,4-Trimethylpentane		Ethylene		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/23/97	19:38	19230242		0.136		1.044		1.978		1.009	3.457	1.309		0.486		0.164		0.546		6.274
9/23/97	19:39	19230243		0.136		1.049		1.987		1.014	3.516	1.314		0.488		0.164		0.549		6.284
9/23/97	20:13	19230262		0.091	3.090	0.401	4.675	0.562	7.591	0.522		0.668		0.382	0.234	0.069	3.001	0.417		4.210
9/23/97	20:15	19230263		0.119	2.453	0.452		1.787	2.520	0.634		1.197		0.439		0.129	1.755	0.479		5.486
9/23/97	20:17	19230264		0.129		1.000		1.894		0.967		1.399		0.466		0.151	1.242	0.507		5.955
9/23/97	20:18	19230265		0.133		1.023		1.937		0.989		1.471		0.476		0.159	1.098	0.519		6.136
9/23/97	20:20	19230266		0.134		1.034		1.960		1.000	3.401	1.294		0.482		0.162		0.541		6.204
9/23/97	20:22	19230267		0.135		1.039		1.967		1.004	3.482	1.307		0.484		0.164		0.544		6.225
9/23/97	20:24	19230268		0.134		1.041		1.973		1.007	3.535	1.309		0.485		0.164		0.545		6.218
9/23/97	20:25	19230269		0.134		1.042		1.974		1.007	3.531	1.311		0.485		0.164		0.545		6.223
9/23/97	20:27	19230270		0.135		1.042		1.974		1.008	3.503	1.311		0.485		0.164		0.545		6.227
9/23/97	20:29	19230271		0.135		1.042		1.974		1.007	3.453	1.309		0.485		0.164		0.545		6.249
9/23/97	20:31	19230272		0.135		1.041		1.972		1.007	3.417	1.307		0.485		0.164		0.545		6.245
9/23/97	20:32	19230273		0.135		1.039		1.969		1.005		1.507		0.484		0.163		0.544		6.246
9/23/97	20:34	19230274		0.135		1.039		1.969		1.005		1.501		0.484		0.162		0.544		6.254
9/23/97	20:36	19230275		0.135		1.039		1.969		1.005		1.504		0.484		0.163		0.544		6.249
9/23/97	20:38	19230276		0.135		1.039		1.968		1.005		1.504		0.484		0.163		0.544		6.260
9/23/97	20:39	19230277		0.136		1.043		1.976		1.008		1.511		0.486		0.163		0.546		6.278
Average ---->				0.137		0.347	1.005	0.197	1.972	0.448	1.009	2.761	1.313	0.497	0.016	0.159	0.401	0.555	0.185	6.334

TABLE E-3. RESULTS FROM APP COATINGS ROOF STACKS

Date	Time	File name	Hexane		Methane		Carbon monoxide	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/24/97 Run 1	12:20	19240001		0.67	3.1	0.38	14.0	3.5
	12:22	19240002		0.72	3.2	0.40	13.6	3.8
	12:23	19240003	1.5	0.52	3.4	0.41	11.4	3.9
	12:25	19240004	1.6	0.53	3.4	0.41	11.5	4.0
	12:27	19240005	1.7	0.53	3.4	0.41	11.8	4.0
	12:29	19240006	1.7	0.52	3.3	0.41	11.4	3.9
	12:30	19240007	1.7	0.52	3.3	0.41	13.0	3.9
	12:32	19240008	1.8	0.52	3.4	0.40	13.5	3.9
	12:34	19240009	1.8	0.52	3.3	0.40	10.6	3.9
	12:36	19240010	1.9	0.52	3.3	0.40	10.9	3.9
	12:38	19240011	1.9	0.51	3.2	0.40	11.3	3.9
	12:39	19240012	2.0	0.52	3.2	0.40	10.8	4.0
	12:41	19240013	2.0	0.52	3.4	0.41	13.3	4.0
	12:43	19240014	2.0	0.52	3.4	0.41	13.7	4.0
	12:45	19240015	2.1	0.53	3.4	0.41	13.9	4.0
	12:46	19240016	2.1	0.53	3.5	0.41	15.9	4.0
	12:48	19240017	1.9	0.53	3.5	0.41	18.2	4.0
	12:50	19240018	1.9	0.52	3.6	0.41	21.9	3.9
	12:52	19240019	2.1	0.53	4.0	0.41	44.3	4.1
	12:54	19240020	2.1	0.52	3.7	0.41	28.9	4.0
	12:55	19240021	2.0	0.53	3.6	0.41	29.3	4.0
	12:57	19240022	2.0	0.53	3.5	0.41	34.7	4.1
	12:59	19240023	2.0	0.54	3.6	0.42	43.6	4.2
	13:01	19240024	2.1	0.53	3.6	0.41	33.3	4.1
	13:02	19240025	2.0	0.53	3.7	0.41	38.0	4.0
	13:04	19240026	1.9	0.53	3.7	0.41	39.8	4.0
	13:06	19240027	1.8	0.53	3.5	0.41	30.4	3.9
	13:08	19240028	1.8	0.54	3.4	0.42	23.4	4.0
	13:09	19240029	1.8	0.54	3.4	0.42	20.1	4.0
	13:11	19240030	1.9	0.54	3.7	0.42	18.9	4.0
	13:13	19240031	1.9	0.54	3.8	0.42	17.9	4.0
	13:15	19240032	1.9	0.54	3.8	0.42	16.1	4.0
	13:17	19240033	1.9	0.54	3.7	0.42	14.6	4.0
	13:18	19240034	2.0	0.54	3.6	0.42	13.5	4.0
	13:20	19240035	1.9	0.54	3.5	0.42	13.5	4.0
	13:22	19240036	1.9	0.54	3.5	0.42	13.1	4.0
	13:24	19240037	1.9	0.55	3.6	0.43	23.2	4.1
	13:25	19240038	1.9	0.55	4.0	0.43	56.3	4.2
	13:27	19240039	1.8	0.56	3.8	0.43	42.7	4.2
	13:29	19240040	1.8	0.56	3.8	0.44	42.5	4.2
	13:31	19240041	1.8	0.56	3.9	0.44	53.5	4.3
	13:33	19240042	1.9	0.56	3.8	0.43	44.4	4.2

TABLE E-3. (continued)

Date	Time	File name	Hexane		Methane		Carbon monoxide	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
	13:34	19240043	1.9	0.55	3.7	0.43	40.6	4.1
	13:36	19240044	1.9	0.55	3.7	0.43	38.9	4.1
Average --->			1.8	0.54	3.5	0.42	24.0	4.0

TABLE E-3. (continued)

Date	Time	File name	Hexane		Methane		Carbon monoxide	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/24/97 Run 2	14:11	19240064	1.8	0.54	3.2	0.42	7.4	3.7
	14:13	19240065	2.0	0.56	3.3	0.44	23.3	3.9
	14:15	19240066	2.0	0.56	3.3	0.44	23.1	4.0
	14:17	19240067	2.3	0.56	3.3	0.44	21.9	4.0
	14:19	19240068	2.4	0.56	3.4	0.43	24.6	4.0
	14:20	19240069	2.3	0.56	3.4	0.44	20.6	4.0
	14:22	19240070	2.4	0.56	3.5	0.44	18.4	4.0
	14:24	19240071	2.6	0.56	3.7	0.44	29.1	4.1
	14:26	19240072	2.4	0.57	3.6	0.44	25.4	4.1
	14:27	19240073	2.4	0.57	3.7	0.44	31.6	4.1
	14:29	19240074	2.4	0.57	3.5	0.45	26.8	4.0
	14:31	19240075	2.4	0.57	3.4	0.45	24.9	4.0
	14:33	19240076	2.2	0.57	3.3	0.45	24.9	4.0
	14:34	19240077	2.1	0.57	3.2	0.44	21.0	3.9
	14:36	19240078	2.2	0.56	3.2	0.44	24.8	3.9
	14:38	19240079	2.2	0.56	3.2	0.44	28.8	3.9
	14:40	19240080	2.2	0.56	3.2	0.44	29.8	3.9
	14:42	19240081	2.5	0.56	3.2	0.44	28.3	3.9
	14:43	19240082	2.5	0.56	3.2	0.44	27.5	4.0
	14:45	19240083	2.3	0.56	3.2	0.44	25.6	3.9
	14:47	19240084	2.3	0.56	3.1	0.44	22.1	3.9
	14:49	19240085	2.3	0.56	3.1	0.44	22.5	3.9
	14:50	19240086	2.2	0.56	3.1	0.44	26.4	3.9
	14:52	19240087	2.1	0.56	3.0	0.44	22.3	3.8
	14:54	19240088	2.1	0.56	3.0	0.44	24.1	3.8
	14:56	19240089	2.0	0.56	3.0	0.44	21.9	3.8
	14:57	19240090	2.0	0.56	3.0	0.44	17.1	3.8
	14:59	19240091	2.0	0.56	3.0	0.44	16.3	3.8
	15:01	19240092	2.0	0.56	3.1	0.43	17.4	3.7
	15:03	19240093	1.9	0.55	3.3	0.43	23.9	3.7
	15:05	19240094	2.1	0.55	3.3	0.43	20.3	3.8
	15:06	19240095	2.0	0.55	3.3	0.43	17.2	3.9
	15:08	19240096	1.9	0.55	3.3	0.43	16.0	3.8
	15:10	19240097	1.9	0.55	3.3	0.43	19.5	3.8
Average →			2.2	0.56	3.3	0.44	22.8	3.9

TABLE E-3. (continued)

Date	Time	File name	Hexane		Methane		Carbon monoxide	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/24/97	15:12	19240098	1.9	0.56	3.4	0.44	23.3	3.8
	15:13	19240099	1.9	0.56	3.3	0.44	23.4	3.8
Run 3	15:15	19240100	1.8	0.56	3.4	0.44	28.2	3.8
	15:17	19240101	1.8	0.56	3.3	0.44	26.1	3.8
	15:19	19240102	1.8	0.57	3.3	0.44	21.5	3.8
	15:21	19240103	1.9	0.56	3.4	0.44	27.8	3.8
	15:22	19240104	2.0	0.56	3.9	0.44	23.6	3.8
	15:24	19240105	2.0	0.56	4.1	0.44	21.7	3.8
	15:26	19240106	1.8	0.55	3.8	0.43	21.6	3.7
	15:28	19240107	1.8	0.55	3.5	0.43	19.5	3.7
	15:29	19240108	1.9	0.55	3.4	0.43	29.4	3.7
	15:31	19240109	1.8	0.55	3.2	0.43	26.6	3.7
	15:33	19240110	1.6	0.55	3.1	0.43	20.1	3.6
	15:35	19240111	1.7	0.55	3.0	0.43	19.6	3.6
	15:36	19240112	1.6	0.55	2.8	0.43	16.2	3.5
	15:38	19240113	1.5	0.54	2.8	0.42	12.6	3.5
	15:40	19240114	1.6	0.54	2.9	0.42	10.7	3.5
	15:42	19240115	1.6	0.54	2.8	0.42	9.6	3.5
	15:44	19240116	1.6	0.54	2.8	0.42	9.0	3.4
	15:45	19240117	1.7	0.54	2.9	0.42	8.6	3.4
	15:47	19240118	1.6	0.54	2.8	0.42	8.1	3.4
	15:49	19240119	1.7	0.54	2.8	0.42	8.2	3.4
	15:51	19240120	1.6	0.54	2.8	0.42	8.0	3.4
	15:52	19240121	1.6	0.54	2.7	0.42	7.8	3.4
	15:54	19240122	1.5	0.54	2.8	0.42	7.6	3.4
	15:56	19240123	1.5	0.54	2.8	0.42	7.7	3.4
	15:58	19240124	1.5	0.54	2.7	0.42	7.9	3.4
	15:59	19240125	1.4	0.55	2.7	0.43	7.9	3.4
	16:01	19240126	1.4	0.55	2.7	0.43	8.0	3.4
	16:03	19240127	1.5	0.55	2.7	0.43	7.9	3.4
	16:05	19240128	1.6	0.55	2.8	0.43	8.0	3.4
	16:07	19240129	1.5	0.55	2.7	0.43	7.9	3.5
	16:08	19240130	1.5	0.55	2.7	0.43	8.0	3.4
	16:10	19240131	1.4	0.55	2.8	0.43	8.0	3.4
	16:12	19240132	1.3	0.55	2.8	0.43	8.1	3.4
	16:14	19240133	1.3	0.55	2.7	0.43	7.9	3.4
	16:15	19240134	1.3	0.55	2.8	0.43	8.0	3.4
	16:17	19240135	1.3	0.56	2.8	0.44	8.1	3.5
	16:19	19240136	1.3	0.56	2.7	0.44	8.1	3.5
	16:21	19240137	1.3	0.56	2.8	0.44	8.3	3.5
	16:22	19240138	1.3	0.56	2.7	0.44	8.2	3.5
	16:24	19240139	1.3	0.56	2.7	0.44	8.3	3.4
	16:26	19240140	1.4	0.56	2.7	0.44	8.5	3.5

TABLE E-3. (continued)

Date	Time	File name	Hexane		Methane		Carbon monoxide	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
	16:28	19240141	1.4	0.56	2.8	0.44	8.4	3.5
	16:30	19240142	1.4	0.56	2.7	0.44	8.8	3.5
	16:31	19240143	1.2	0.56	2.7	0.44	8.5	3.5
	16:33	19240144		0.56	2.6	0.44	8.1	3.4
	16:35	19240145		0.57	2.9	0.44	8.2	3.4
	16:37	19240146		0.57	2.7	0.44	8.1	3.4
	16:38	19240147		0.56	2.7	0.44	8.2	3.3
	18:12	insp07	1.5	0.23	3.2	0.37	21.9	2.8
	18:14	insp08	1.5	0.23	3.6	0.37	20.5	2.8
	18:16	insp09	1.6	0.23	3.3	0.37	20.2	2.8
Average --->			1.5	0.55	3.0	0.43	13.1	3.5

TABLE E-4. RESULTS FROM SBS COATER ROOF STACK

Date	Time	File name	Hexane		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/24/97	13:38:	19240045	1.9	0.54	3.6	0.42	32.9	4.0
9/24/97	13:40:	19240046	1.6	0.52	3.3	0.40	17.2	3.7
9/24/97	13:41:	19240047	1.5	0.51	3.3	0.40	8.7	3.6
9/24/97	13:43:	19240048	1.4	0.51	3.4	0.40		3.8
9/24/97	13:45:	19240049	1.4	0.52	3.4	0.40		3.8
9/24/97	13:47:	19240050	1.4	0.52	3.3	0.41		3.8
9/24/97	13:48:	19240051	1.3	0.52	3.2	0.41		3.8
9/24/97	13:50:	19240052	1.3	0.52	3.2	0.41		3.8
9/24/97	13:52:	19240053	1.3	0.52	3.1	0.40		3.8
9/24/97	13:54:	19240054	1.4	0.52	3.0	0.40		3.8
9/24/97	13:56:	19240055	1.4	0.51	3.0	0.40		3.8
9/24/97	13:57:	19240056	1.4	0.51	3.0	0.40		3.8
9/24/97	13:59:	19240057	1.4	0.51	3.1	0.40		3.8
9/24/97	14:1:	19240058	1.5	0.51	3.1	0.40		3.8
9/24/97	14:3:	19240059	1.5	0.51	3.1	0.40		3.8
9/24/97	14:4:	19240060	1.4	0.52	3.1	0.40		3.8
9/24/97	14:6:	19240061	1.4	0.52	3.1	0.41		3.8
9/24/97	14:8:	19240062	1.4	0.52	3.1	0.41		3.8
9/24/97	14:10:	19240063	1.4	0.52	3.2	0.41		3.8
9/25/97	8:25:	19250003	1.5	0.16	3.0	0.25		2.5
9/25/97	8:27:	19250004	1.7	0.17	3.5	0.27	6.0	2.6
9/25/97	8:29:	19250005	1.8	0.18	3.6	0.28	6.8	2.7
9/25/97	8:31:	19250006	1.8	0.18	3.6	0.29	7.9	2.7
9/25/97	8:32:	19250007	1.9	0.18	3.6	0.29	8.7	2.7
9/25/97	8:34:	19250008	1.9	0.18	3.6	0.29	8.4	2.7
9/25/97	8:36:	19250009	1.9	0.18	3.6	0.29	8.3	2.7
9/25/97	8:38:	19250010	1.9	0.18	3.6	0.29	8.0	2.7
9/25/97	8:40:	19250011	2.0	0.18	3.6	0.29	8.9	2.7
9/25/97	8:41:	19250012	2.0	0.18	3.5	0.29	8.7	2.7
9/25/97	8:43:	19250013	2.0	0.18	3.5	0.29	7.4	2.7
9/25/97	8:45:	19250014	2.0	0.18	3.4	0.29	6.8	2.7
9/25/97	8:47:	19250015	2.0	0.18	3.4	0.29	7.4	2.7
9/25/97	8:48:	19250016	2.0	0.18	3.6	0.30	8.1	2.7
9/25/97	8:50:	19250017	2.0	0.19	3.5	0.30	8.7	2.7
9/25/97	8:52:	19250018	2.0	0.19	3.5	0.30	10.0	2.7
9/25/97	8:54:	19250019	2.0	0.19	3.3	0.30	8.2	2.6
9/25/97	8:56:	19250020	2.0	0.19	3.5	0.31	7.5	2.7
9/25/97	8:57:	19250021	2.0	0.19	3.6	0.31	7.1	2.7
9/25/97	8:59:	19250022	2.0	0.19	3.4	0.30	6.5	2.6
9/25/97	9:1:	19250023	2.0	0.19	3.4	0.30	6.7	2.6
9/25/97	9:3:	19250024	2.0	0.19	3.7	0.30	16.3	2.7
9/25/97	9:4:	19250025	2.1	0.19	3.8	0.31	17.7	2.7
9/25/97	9:6:	19250026	2.1	0.19	3.7	0.31	14.6	2.7
9/25/97	9:8:	19250027	2.1	0.19	3.6	0.31	14.2	2.7
9/25/97	9:10:	19250028	2.1	0.19	3.6	0.31	22.9	2.7
9/25/97	9:11:	19250029	2.1	0.19	3.4	0.31	16.8	2.7
9/25/97	9:13:	19250030	2.1	0.20	3.7	0.31	17.6	2.7

TABLE E-4. (continued)

Date	Time	File name	Hexane		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/25/97	9:15:	19250031	2.1	0.20	3.8	0.32	25.1	2.7
9/25/97	9:17:	19250032	2.2	0.20	4.4	0.32	46.5	2.9
9/25/97	9:19:	19250033	2.2	0.20	4.0	0.32	28.3	2.7
9/25/97	9:20:	19250034	2.1	0.20	3.9	0.32	24.2	2.7
9/25/97	9:22:	19250035	2.2	0.20	3.8	0.32	19.9	2.7
9/25/97	9:24:	19250036	2.1	0.20	3.6	0.32	14.2	2.7
9/25/97	9:26:	19250037	2.1	0.20	3.9	0.32	27.3	2.7
9/25/97	9:27:	19250038	2.2	0.20	3.8	0.32	27.3	2.7
9/25/97	9:29:	19250039	2.1	0.20	3.7	0.32	18.2	2.7
9/25/97	9:40:	19250045	2.2	0.20	3.8	0.33	19.6	2.7
9/25/97	9:42:	19250046	2.2	0.20	3.7	0.33	20.1	2.7
9/25/97	9:43:	19250047	2.2	0.20	3.9	0.33	29.5	2.7
9/25/97	9:45:	19250048	2.2	0.20	3.8	0.33	26.1	2.7
9/25/97	9:47:	19250049	2.2	0.20	3.7	0.33	17.8	2.7
9/25/97	9:49:	19250050	2.2	0.21	3.5	0.33	13.8	2.7
9/25/97	9:50:	19250051	2.2	0.21	3.6	0.33	18.3	2.7
9/25/97	9:52:	19250052	2.2	0.21	3.6	0.34	15.8	2.7
9/25/97	9:54:	19250053	2.2	0.21	3.5	0.34	20.0	2.7
9/25/97	9:56:	19250054	2.2	0.21	3.3	0.34	17.2	2.7
9/25/97	9:58:	19250055	2.1	0.21	3.3	0.34	11.9	2.6
9/25/97	9:59:	19250056	2.2	0.21	3.3	0.34	13.9	2.6
9/25/97	10:1:	19250057	2.2	0.21	3.4	0.34	13.7	2.6
9/25/97	10:3:	19250058	2.2	0.21	3.8	0.34	30.1	2.7
9/25/97	10:5:	19250059	2.2	0.21	3.7	0.34	28.5	2.7
9/25/97	10:6:	19250060	2.2	0.21	3.5	0.34	19.3	2.7
9/25/97	10:8:	19250061	2.3	0.21	3.7	0.34	23.5	2.7
9/25/97	10:10:	19250062	2.2	0.21	3.6	0.34	16.4	2.7
9/25/97	10:12:	19250063	2.3	0.21	3.7	0.34	25.4	2.7
9/25/97	10:13:	19250064	2.3	0.22	3.6	0.35	22.5	2.7
9/25/97	10:15:	19250065	2.3	0.22	3.3	0.35	14.2	2.7
9/25/97	10:17:	19250066	2.3	0.22	3.0	0.35	12.4	2.6
9/25/97	10:19:	19250067	2.4	0.22	3.2	0.35	14.8	2.7
9/25/97	10:20:	19250068	2.4	0.22	3.7	0.35	27.3	2.7
9/25/97	10:22:	19250069	2.4	0.22	3.6	0.35	20.2	2.7
9/25/97	10:24:	19250070	2.4	0.22	3.5	0.35	15.8	2.7
9/25/97	10:26:	19250071	2.5	0.22	3.6	0.35	18.7	2.7
9/25/97	10:27:	19250072	2.5	0.22	3.6	0.35	19.4	2.7
9/25/97	10:29:	19250073	2.5	0.22	3.7	0.35	33.3	2.8
9/25/97	10:31:	19250074	2.5	0.22	3.4	0.35	23.9	2.7
9/25/97	10:33:	19250075	2.4	0.22	3.4	0.35	19.3	2.7
9/25/97	10:35:	19250076	2.4	0.22	3.6	0.36	19.7	2.7
9/25/97	10:36:	19250077	2.4	0.22	3.6	0.36	23.0	2.7
9/25/97	10:38:	19250078	2.4	0.22	3.8	0.36	38.1	2.8
9/25/97	10:40:	19250079	2.4	0.22	3.5	0.36	21.3	2.7
9/25/97	10:42:	19250080	2.4	0.22	3.6	0.36	21.2	2.7
9/25/97	10:43:	19250081	2.4	0.22	3.6	0.36	19.5	2.7
9/25/97	10:45:	19250082	2.4	0.22	3.4	0.36	13.7	2.6

TABLE E-4. (continued)

Date	Time	File name	Hexane		Methane		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/25/97	10:47:	19250083	2.4	0.22	3.4	0.36	21.2	2.6
9/24/97	18:29:	outsp10	1.0	0.46	3.5	0.36	10.5	2.7
9/24/97	18:31:	outsp11	1.0	0.46	3.5	0.36	10.3	2.7
9/24/97	18:33:	outsp12	1.1	0.43	3.3	0.34	10.4	2.7
9/25/97	11:26:	SBSSP01	2.0	0.21	4.0	0.34	31.8	2.3
9/25/97	11:30:	SBSSP02	1.9	0.21	3.9	0.33	28.1	2.3
9/25/97	11:32:	SBSSP03	1.9	0.21	3.9	0.33	21.7	2.3
Average --->			2.0	0.26	3.5	0.34	14.4	2.9

TABLE E-5. RESULTS FROM APP MIXING TANK

Date	Time	File name	Carbonyl sulfide		Methanol		Ethylene		Sulfur dioxide		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/25/97	13:06	19250097	0.53	0.080	0.10	0.01	1.2	0.3	8.5		40.0	3.5
	13:08	19250098	0.55	0.081	0.10	0.01	1.2	0.3	8.8		42.7	3.6
	13:09	19250099	0.54	0.082	0.10	0.01	1.2	0.3	9.0		45.9	3.6
	13:11	19250100	0.55	0.082	0.11	0.01	1.2	0.3	9.2		49.3	3.6
	13:13	19250101	0.57	0.083	0.11	0.01	1.2	0.3	9.5		52.2	3.7
	13:15	19250102	0.58	0.084	0.11	0.01	1.2	0.3	9.7		55.2	3.7
	13:16	19250103	0.58	0.083	0.11	0.01	1.2	0.3	9.8		55.7	3.7
	13:18	19250104	0.59	0.083	0.12	0.01	1.2	0.4	10.0		55.1	3.7
	13:20	19250105	0.63	0.084	0.12	0.01	1.3	0.4	10.4		55.5	3.7
	13:22	19250106	0.63	0.085	0.12	0.01	1.3	0.4	10.5		56.6	3.7
	13:24	19250107	0.63	0.085	0.12	0.01	1.3	0.4	10.5		58.5	3.7
	13:25	19250108	0.63	0.086	0.12	0.01	1.3	0.4	10.7		61.0	3.8
	13:27	19250109	0.64	0.086	0.12	0.01	1.4	0.4	10.9		62.7	3.8
	13:29	19250110	0.65	0.086	0.13	0.01	1.4	0.4	11.1		62.4	3.8
	13:31	19250111	0.67	0.087	0.13	0.01	1.4	0.4	11.3		61.1	3.8
	13:32	19250112	0.66	0.086	0.13	0.01	1.4	0.4	11.4		60.0	3.8
	13:34	19250113	0.69	0.087	0.13	0.01	1.4	0.4	11.8		58.8	3.8
	13:36	19250114	0.70	0.087	0.13	0.01	1.4	0.4	12.0		58.6	3.9
	13:38	19250115	0.73	0.088	0.14	0.01	1.5	0.4	12.4		59.6	3.9
	13:39	19250116	0.75	0.089	0.14	0.01	1.5	0.5	12.8		60.5	3.9
	13:41	19250117	0.75	0.089	0.14	0.01	1.5	0.5	13.0		61.9	3.9
	13:43	19250118	0.78	0.090	0.15	0.01	1.5	0.5	13.5		64.1	4.0
	13:45	19250119	0.79	0.091	0.15	0.01	1.5	0.5	13.8		65.1	4.0
	13:47	19250120	0.79	0.092	0.15	0.01	1.5	0.5	14.0		65.6	4.0
	13:48	19250121	0.79	0.092	0.15	0.01	1.5	0.5	14.1		67.5	4.1
	13:50	19250122	0.79	0.092	0.15	0.01	1.5	0.5	14.2		68.5	4.1
	13:52	19250123	0.80	0.093	0.16	0.01	1.6	0.5	14.4		68.0	4.1
	13:54	19250124	0.80	0.092	0.16	0.01	1.5	0.5	14.4		66.7	4.1
	13:55	19250125	0.81	0.092	0.16	0.01	1.5	0.5	14.5		65.0	4.1
	13:57	19250126	0.83	0.093	0.16	0.01	1.5	0.5	14.9		63.1	4.1
	13:59	19250127	0.85	0.094	0.16	0.01	1.6	0.5	15.1		61.2	4.1
	14:01	19250128	0.88	0.094	0.17	0.01	1.6	0.5	15.5		60.1	4.2
	14:02	19250129	0.89	0.094	0.17	0.01	1.6	0.6	15.7		59.7	4.2

TABLE E-5. (continued)

Date	Time	File name	Carbonyl sulfide		Methanol		Ethylene		Sulfur dioxide		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
	14:04	19250130	0.91	0.095	0.17	0.01	1.6	0.6	16.1		60.1	4.2
	14:06	19250131	0.90	0.094	0.17	0.01	1.6	0.6	16.0		58.5	4.2
	14:08	19250132	0.88	0.093	0.17	0.01	1.8	0.6	32.3	15.8	56.6	4.1
	14:10	19250133	0.87	0.092	0.16	0.01	1.8	0.6	33.2	15.7	54.8	4.1
	14:11	19250134	0.85	0.091	0.16	0.01	1.7	0.6	34.1	15.6	53.6	4.0
	14:13	19250135	0.85	0.091	0.16	0.01	1.7	0.6	35.2	15.5	52.9	4.0
	14:15	19250136	0.84	0.091	0.16	0.01	1.7	0.6	35.8	15.4	53.3	4.0
	14:17	19250137	0.89	0.093	0.17	0.01	1.8	0.6	36.6	16.2	55.5	4.1
	14:18	19250138	0.94	0.094	0.17	0.01	1.9	0.6	37.4	16.8	57.4	4.1
	14:20	19250139	0.99	0.096	0.18	0.01	2.0	0.6	38.5	17.6	58.8	4.2
Average --->			0.74	0.089	0.14	0.01	1.49	0.46	6.59	12.98	58.35	3.93

TABLE E-6. SBS MIXING TANK 11

Date	Time	File name	Carbonyl sulfide		Hexane		Methane		Sulfur dioxide		CO		Ammonia	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/25/97	17:05	19250146	0.14	0.06	44.13	0.56	4.99	0.51	107.49	6.80	14.44	2.44		1.31
	17:07	19250147	0.15	0.06	48.75	0.65	5.22	0.58	118.14	7.38	11.94	2.67		1.43
	17:09	19250148	0.12	0.06	46.52	0.63	4.83	0.57	115.49	7.18	9.75	2.66		1.39
	17:11	19250149		0.06	37.90	0.56	3.61	0.51	106.55	6.57	6.27	2.50		1.27
	17:12	19250150		0.06	41.08	0.60	4.58	0.55	101.28	6.25	7.80	2.64	2.66	1.26
	17:14	19250151	0.13	0.06	43.45	0.64	4.93	0.58	99.15	6.14	8.66	2.72	3.11	1.24
	17:16	19250152	0.13	0.06	43.54	0.66	4.82	0.60	96.13	5.94	8.61	2.73	3.34	1.20
	17:18	19250153	0.12	0.06	42.74	0.68	4.60	0.62	91.67	5.66	8.51	2.72	3.48	1.14
	17:20	19250154		0.06	41.99	0.70	4.52	0.63	86.98	5.35	7.95	2.74	3.62	1.08
	17:21	19250155		0.06	40.75	0.71	4.40	0.64	82.33	5.06	8.19	2.72	3.74	1.02
	17:23	19250156		0.06	39.25	0.71	4.37	0.64	77.81	4.78	8.06	2.71	3.81	0.97
	17:25	19250157		0.06	38.49	0.71	4.24	0.65	74.27	4.58	7.73	2.69	3.96	0.93
	17:27	19250158		0.06	37.64	0.71	4.06	0.65	71.84	4.43	7.28	2.68	4.06	0.90
	17:28	19250159		0.06	37.04	0.71	4.09	0.64	70.40	4.35	7.03	2.68	4.23	0.88
	17:30	19250160		0.06	36.16	0.70	4.08	0.64	68.92	4.27	6.85	2.66	4.28	0.86
	17:32	19250161		0.06	36.20	0.71	4.05	0.64	67.88	4.20	6.75	2.68	4.31	0.85
	17:34	19250162		0.06	35.97	0.71	4.04	0.64	66.88	4.15	6.83	2.68	4.33	0.84
	17:35	19250163		0.06	35.62	0.70	4.06	0.64	66.02	4.11	6.90	2.66	4.37	0.83
	17:37	19250164		0.06	35.77	0.71	4.33	0.64	65.35	4.10	7.22	2.68	4.57	0.83
	17:39	19250165		0.06	35.21	0.70	4.18	0.64	65.14	4.08	7.11	2.66	4.60	0.82
	17:41	19250166		0.06	35.20	0.70	4.08	0.64	65.16	4.07	7.17	2.65	4.63	0.82
	17:43	19250167		0.06	34.83	0.70	4.09	0.64	64.73	4.04	7.24	2.65	4.69	0.82
	17:44	19250168		0.06	34.60	0.70	4.03	0.63	64.16	4.00	7.06	2.63	4.72	0.81
	17:46	19250169		0.06	34.60	0.69	3.97	0.63	63.75	4.00	6.93	2.63	4.76	0.81
	17:48	19250170		0.06	35.05	0.70	4.10	0.63	63.77	4.01	7.24	2.64	4.98	0.81
	17:50	19250171		0.06	34.81	0.69	4.02	0.63	63.29	4.00	7.31	2.63	5.05	0.81
	17:51	19250172		0.06	35.52	0.70	4.02	0.64	63.42	3.99	11.12	2.65	5.16	0.81
	17:53	19250173		0.06	36.92	0.71	4.13	0.65	64.50	4.05	13.57	2.69	5.47	0.82
	17:55	19250174		0.06	37.41	0.72	4.23	0.65	64.91	4.10	10.66	2.69	5.72	0.83
	17:57	19250175		0.06	37.23	0.71	4.19	0.65	65.50	4.12	9.05	2.68	5.74	0.83
	17:58	19250176		0.06	37.04	0.71	4.25	0.64	65.52	4.12	12.01	2.68	5.80	0.83
	18:00	19250177		0.06	37.30	0.71	4.24	0.64	66.06	4.16	18.44	2.69	6.00	0.84
	18:02	19250178		0.06	37.30	0.71	4.18	0.64	66.61	4.19	17.02	2.69	6.03	0.85
	18:21	T11SP01		0.05	25.47	0.58	3.96	0.53	47.74	3.12	33.49	2.27	3.96	0.63
	18:24	T11SP02		0.05	24.56	0.59	3.90	0.54	46.77	3.08	32.19	2.27	3.93	0.62
	18:26	T11SP03		0.05	24.63	0.60	3.94	0.55	46.63	3.07	34.70	2.29	4.04	0.62
Average ---->			0.02	0.06	38.36	0.68	4.29	0.62	77.0	4.8	9.1	2.7	4.0	0.96

TABLE E-7. RESULTS FROM APP HOLDING TANK 1

Date	Time	File name	Benzene		Carbonyl sulfide		Ethylene dichloride		Methanol		Hexane		Propionaldehyde		Sulfur dioxide		CO		Ammonia		Formaldehyde	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/26/97	16:8	APP01			1.9	0.091	5.0	1.7	0.029	0.005					174.2	5.9	220.5	4.0	6.3	1.04		
	16:17	APP02			1.9	0.090	5.4	1.8	0.035	0.005					169.3	6.1	219.3	4.0	6.1	1.1		
	16:21	APP03			0.52	0.047	2.7	1.1	0.028	0.003					60.6	3.8	85.7	2.1	3.3	0.62		
	16:25	APP04*	10.7	2.0	0.11	0.033		0.47	0.015	0.001	16.5	1.3	16.0	2.0	16.9	1.6	19.3	1.4	1.7	0.30	21.7	1.5
		Dilution Corrected APP04	65.9		0.7				0.1		101.6		98.7		104.1		118.7		10.4		133.6	
	16:48	APP05			1.0	0.070	8.7	1.5	0.054	0.004					55.0	5.4	90.9	3.1	6.4	0.91		
	17:6	APP06			2.5	0.076	21.7	3.4	0.10	0.010					103.5	12.1	132.0	3.4	20.5	2.0		
	17:10	APP07			2.7	0.084	22.7	3.5	0.11	0.010					100.5	12.3	135.6	3.7	22.7	2.1		
Average --->			65.9	2.0	1.6	0.1	9.5	1.9	0.1	0.0	101.6	1.3	98.7	2.0	109.6	6.7	143.2	3.1	10.8	1.1	133.6	1.5

TABLE E-8. RESULTS FROM SBS HOLDING TANK 3

Date	Time	File name	Carbonyl sulfide				Methanol				Propane		Hexane		Propionaldehyde		Styrene		1,1,2,2-Tetrachloroethane	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/26/97	10:17	19260007	0.85	0.11		0.0028	11.94	0.83	75.9	1.1	23.6	1.8		1.25		0.56		1.2	20.2	0.89
9/26/97	10:19	19260008	0.96	0.11		0.0025	13.42	0.89	79.8	1.2	26.1	1.9		1.15		0.51		1.1	22.0	0.95
9/26/97	10:20	19260009	0.99	0.11		0.0024	13.05	0.91	80.7	1.2	26.9	1.9		1.08		0.48		1.0	22.2	0.97
9/26/97	10:22	19260010	0.98	0.11		0.0023	12.50	0.89	78.8	1.2	26.8	1.9		1.02		0.46		0.99	21.9	0.95
9/26/97	10:24	19260011	0.95	0.11		0.0022	11.31	0.86	76.1	1.2	26.1	1.9		0.97		0.43		0.95	21.0	0.93
9/26/97	10:26	19260012	0.92	0.11	0.0059	0.0019	10.40	0.85	74.1	1.2	25.8	1.8	2.9	0.82		0.42		0.92	20.3	0.91
9/26/97	10:28	19260013	0.90	0.11	0.0062	0.0018	9.61	0.82	71.4	1.1	25.2	1.8	2.8	0.80		0.41		0.90	19.6	0.88
9/26/97	10:29	19260014	0.87	0.11	0.0066	0.0018	8.73	0.80	68.9	1.1	24.6	1.7	2.6	0.78		0.40		0.88	18.8	0.85
9/26/97	10:31	19260015	0.84	0.11	0.0067	0.0018	7.96	0.78	66.8	1.1	24.2	1.7	2.5	0.78		0.40		0.87	18.1	0.83
9/26/97	10:33	19260016	0.82	0.10	0.0068	0.0018	7.36	0.76	65.2	1.0	23.8	1.6	2.4	0.77		0.40		0.87	17.6	0.82
9/26/97	10:35	19260017	0.80	0.10	0.0069	0.0018	6.81	0.73	62.6	1.0	23.2	1.6	2.3	0.77		0.40		0.86	16.9	0.79
9/26/97	10:36	19260018	0.77	0.10	0.0070	0.0017	6.04	0.71	60.5	0.98	22.6	1.5	2.2	0.76		0.39		0.85	16.2	0.77
9/26/97	10:38	19260019	0.75	0.099	0.0072	0.0018	5.46	0.70	59.4	0.97	22.4	1.5	2.3	0.77		0.39		0.86	15.7	0.75
9/26/97	10:40	19260020	0.74	0.099	0.0073	0.0018	4.97	0.69	58.3	0.95	22.1	1.5	2.2	0.78		0.40		0.86	15.3	0.74
9/26/97	10:42	19260021	0.72	0.098	0.0076	0.0018	4.49	0.68	57.1	0.93	21.8	1.4	2.2	0.78		0.40		0.86	14.8	0.73
9/26/97	10:43	19260022	0.70	0.096	0.0076	0.0017	4.20	0.65	54.7	0.89	21.1	1.4	2.1	0.77		0.39		0.85	14.3	0.70
9/26/97	10:45	19260023	0.69	0.096	0.0077	0.0018	3.51	0.65	54.2	0.89	21.0	1.4	2.0	0.78		0.39		0.85	13.9	0.69
9/26/97	10:47	19260024	0.68	0.095	0.0079	0.0018	3.06	0.64	53.8	0.89	21.0	1.4	1.9	0.79		0.40		0.87	13.6	0.69
9/26/97	10:49	19260025	0.67	0.094	0.0078	0.0018	2.68	0.64	53.2	0.88	20.9	1.4	1.9	0.80		0.40		0.88	13.3	0.68
9/26/97	10:51	19260026	0.66	0.094	0.0088	0.0019	2.3	0.63	52.5	0.87	20.8	1.3	1.7	0.81		0.41		0.89	12.9	0.67
9/26/97	10:52	19260027	0.65	0.093	0.0082	0.0018	2.3	0.61	50.7	0.84	20.2	1.3	1.8	0.81		0.40		0.88	12.6	0.65
9/26/97	10:54	19260028	0.63	0.092	0.0092	0.0019	1.7	0.61	50.6	0.84	20.2	1.3		0.82		0.41		0.89	12.3	0.65
9/26/97	10:56	19260029	0.63	0.092	0.010	0.0019	1.4	0.61	50.3	0.84	20.2	1.3	1.7	0.83		0.41	3.5	0.83	12.0	0.65
9/26/97	10:58	19260030	0.62	0.091	0.011	0.0019	1.3	0.59	49.0	0.82	19.9	1.3		0.83		0.41	3.5	0.83	11.7	0.64
9/26/97	10:59	19260031	0.61	0.090	0.011	0.0019		0.64	49.4	0.72	20.7	1.1		0.83		0.42	3.7	0.84	11.5	0.64
9/26/97	11:01	19260032	0.61	0.089	0.011	0.0019		0.64	48.8	0.71	20.5	1.1		0.84		0.42	3.8	0.84	11.3	0.63
9/26/97	11:03	19260033	0.59	0.089	0.012	0.0020		0.63	48.2	0.70	20.0	1.1		0.84	1.3	0.42	2.7	0.93	11.0	0.62
9/26/97	11:05	19260034	0.59	0.088	0.012	0.0020		0.63	47.9	0.70	19.7	1.1		0.85	1.3	0.43	2.8	0.94	10.8	0.62
9/26/97	11:06	19260035	0.59	0.088	0.012	0.0020		0.62	47.2	0.69	19.5	1.1		0.85	1.3	0.43	2.7	0.94	10.6	0.61
9/26/97	11:08	19260036	0.59	0.088	0.012	0.0020		0.62	46.8	0.69	19.2	1.1		0.85	1.4	0.43	2.8	0.95	10.4	0.61
9/26/97	11:10	19260037	0.58	0.087	0.012	0.0020		0.62	46.8	0.69	19.0	1.1		0.86	1.4	0.43	2.9	0.95	10.2	0.61
9/26/97	11:12	19260038	0.59	0.087	0.013	0.0020		0.61	46.4	0.69	19.0	1.1		0.87	1.4	0.44	3.0	0.96	10.1	0.61
9/26/97	11:14	19260039	0.58	0.087	0.013	0.0020		0.61	46.1	0.69	18.7	1.1		0.87	1.4	0.44	3.1	0.96	9.9	0.61
9/26/97	11:15	19260040	0.58	0.087	0.013	0.0021		0.62	46.4	0.69	18.6	1.1		0.88	1.5	0.44	3.2	0.98	9.8	0.62
9/26/97	11:42	T3SP01	0.47	0.072	0.013	0.0020		0.56	39.9	0.65	16.2	1.0		0.84	2.1	0.37	21.9	0.82	8.0	0.58
9/26/97	11:46	T3SP02	0.35	0.065	0.012	0.0018		0.59	39.2	0.69	11.8	1.1		0.78	1.7	0.34	21.9	0.76	6.7	0.62
Average -->			0.73	0.098	0.0078	0.0020	4.6	0.70	58.2	0.91	21.9	1.4	1.1	0.86	0.32	0.42	1.1	0.92	14.8	0.73

TABLE E-8. (continued)

Date	Time	File name	p-Xylene		Methane		Sulfur dioxide		CO	
			ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty	ppm	Uncertainty
9/26/97	10:17	19260007	46.1	2.9	93.4	4.7	26.1	0.56	9.2	1.2
9/26/97	10:19	19260008	42.8	2.6	105.2	5.0	26.9	0.51	10.1	1.3
9/26/97	10:20	19260009	42.0	2.5	110.3	5.1	27.2	0.48	10.7	1.3
9/26/97	10:22	19260010	38.9	2.3	113.4	5.0	26.6	0.46	10.6	1.3
9/26/97	10:24	19260011	39.5	2.2	114.2	4.9	25.6	0.43	10.4	1.3
9/26/97	10:26	19260012	40.2	2.2	116.1	4.9	24.9	0.42	10.4	1.2
9/26/97	10:28	19260013	41.5	2.1	117.0	4.8	23.8	0.41	10.1	1.2
9/26/97	10:29	19260014	43.1	2.1	117.2	4.7	22.8	0.40	9.9	1.2
9/26/97	10:31	19260015	45.2	2.1	118.3	4.7	21.8	0.40	9.8	1.1
9/26/97	10:33	19260016	47.7	2.1	119.6	4.6	20.8	0.39	9.8	1.1
9/26/97	10:35	19260017	48.8	2.1	119.4	4.6	19.6	0.39	9.4	1.1
9/26/97	10:36	19260018	50.0	2.0	119.0	4.5	18.7	0.39	9.2	1.0
9/26/97	10:38	19260019	52.5	2.0	120.0	4.4	17.9	0.39	9.2	1.0
9/26/97	10:40	19260020	54.8	2.1	120.8	4.4	17.1	0.39	9.2	1.0
9/26/97	10:42	19260021	56.7	2.1	121.2	4.3	16.3	0.40	9.1	1.00
9/26/97	10:43	19260022	56.0	2.0	120.4	4.3	15.3	0.39	8.6	0.95
9/26/97	10:45	19260023	57.8	2.1	120.5	4.2	14.8	0.39	8.6	0.95
9/26/97	10:47	19260024	60.5	2.1	121.4	4.2	14.2	0.40	8.7	0.94
9/26/97	10:49	19260025	62.7	2.1	121.8	4.1	13.6	0.41	8.8	0.94
9/26/97	10:51	19260026	64.1	2.2	121.9	4.1	13.1	0.41	8.7	0.92
9/26/97	10:52	19260027	64.0	2.2	121.5	4.1	12.4	0.41	8.4	0.90
9/26/97	10:54	19260028	65.0	2.2	121.7	4.1	12.1	0.41	8.5	0.90
9/26/97	10:56	19260029	66.4	2.2	122.5	4.1	11.6	0.42	8.6	0.90
9/26/97	10:58	19260030	65.9	2.2	121.9	4.0	11.0	0.42	8.3	0.87
9/26/97	10:59	19260031	67.2	2.2	121.6	4.0	10.8	0.42	8.2	0.86
9/26/97	11:01	19260032	68.1	2.2	122.3	3.9	10.3	0.42	8.2	0.85
9/26/97	11:03	19260033	67.7	2.3	121.5	3.9	10.0	0.43	8.2	0.85
9/26/97	11:05	19260034	68.8	2.3	121.5	3.9	9.7	0.43	8.3	0.84
9/26/97	11:06	19260035	69.2	2.3	121.5	3.9	9.2	0.43	8.2	0.83
9/26/97	11:08	19260036	69.7	2.3	121.0	3.9	8.9	0.43	8.2	0.83
9/26/97	11:10	19260037	70.9	2.3	121.3	3.8	8.8	0.43	8.4	0.83
9/26/97	11:12	19260038	71.6	2.3	122.2	3.8	8.4	0.44	8.3	0.82
9/26/97	11:14	19260039	71.8	2.3	121.4	3.8	8.3	0.44	8.4	0.82
9/26/97	11:15	19260040	73.1	2.4	121.8	3.8	8.1	0.45	8.5	0.83
9/26/97	11:42	T3SP01	66.3	2.3	109.7	3.2	5.1	0.42	7.3	0.78
9/26/97	11:46	T3SP02	62.8	2.1	88.6	2.9	5.4	0.39	6.9	0.83
Average -->			57.4	2.2	118.7	4.3	16.1	0.42	9.0	1.0

APPENDIX F

EPA METHOD 320 AND EPA FTIR PROTOCOL

3. Appendix A of part 63 is amended by adding, in numerical order, Methods 320, 321, and 322 to read as follows:

Appendix A to Part 63-Test Methods

(PROPOSED) TEST METHOD 320

MEASUREMENT OF VAPOR PHASE ORGANIC AND INORGANIC EMISSIONS BY EXTRACTIVE FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY

1.0 Introduction.

Persons unfamiliar with basic elements of FTIR spectroscopy should not attempt to use this method. This method describes sampling and analytical procedures for extractive emission measurements using Fourier transform infrared (FTIR) spectroscopy. Detailed analytical procedures for interpreting infrared spectra are described in the "Protocol for the Use of Extractive Fourier Transform Infrared (FTIR) Spectrometry in Analyses of Gaseous Emissions from Stationary Sources," hereafter referred to as the "Protocol." Definitions not given in this method are given in appendix A of the Protocol. References to specific sections in the Protocol are made throughout this Method. For additional information refer to references 1 and 2, and other EPA reports, which describe the use of FTIR spectrometry in specific field measurement applications and validation tests. The sampling procedure described here is extractive. Flue gas is extracted through a heated gas transport and handling system. For some sources, sample conditioning systems may be applicable. Some examples are given in this method. Note: sample conditioning systems may be used providing the method validation requirements in Sections 9.2 and 13.0 of this method are met.

1.1 Scope and Applicability.

1.1.1 Analytes. Analytes include hazardous air pollutants (HAPs) for which EPA reference spectra have been developed. Other compounds can also be measured with this method if reference spectra are prepared according to section 4.6 of the protocol.

1.1.2 Applicability. This method applies to the analysis of vapor phase organic or inorganic compounds which absorb energy in the mid-infrared spectral region, about 400 to 4000 cm^{-1} (25 to $2.5\text{ }\mu\text{m}$). This method is used to determine compound-specific concentrations in a multi-component vapor phase sample, which is contained in a closed-path gas cell. Spectra of samples are collected using double beam infrared absorption spectroscopy. A computer program is used to analyze spectra and report compound concentrations.

1.2 Method Range and Sensitivity. Analytical range and sensitivity depend on the frequency-dependent analyte absorptivity, instrument configuration, data collection parameters, and gas stream composition. Instrument factors include: (a) spectral resolution, (b) interferometer signal

averaging time, (c) detector sensitivity and response, and (d) absorption path length.

1.2.1 For any optical configuration the analytical range is between the absorbance values of about .01 (infrared transmittance relative to the background = 0.98) and 1.0 ($T = 0.1$). (For absorbance > 1.0 the relation between absorbance and concentration may not be linear.)

1.2.2 The concentrations associated with this absorbance range depend primarily on the cell path length and the sample temperature. An analyte absorbance greater than 1.0, can be lowered by decreasing the optical path length. Analyte absorbance increases with a longer path length. Analyte detection also depends on the presence of other species exhibiting absorbance in the same analytical region. Additionally, the estimated lower absorbance (A) limit ($A = 0.01$) depends on the root mean square deviation (RMSD) noise in the analytical region.

1.2.3 The concentration range of this method is determined by the choice of optical configuration.

1.2.3.1 The absorbance for a given concentration can be decreased by decreasing the path length or by diluting the sample. There is no practical upper limit to the measurement range.

1.2.3.2 The analyte absorbance for a given concentration may be increased by increasing the cell path length or (to some extent) using a higher resolution. Both modifications also cause a corresponding increased absorbance for all compounds in the sample, and a decrease in the signal throughput. For this reason the practical lower detection range (quantitation limit) usually depends on sample characteristics such as moisture content of the gas, the presence of other interferants, and losses in the sampling system.

1.3 Sensitivity. The limit of sensitivity for an optical configuration and integration time is determined using appendix D of the Protocol: Minimum Analyte Uncertainty, (MAU). The MAU depends on the RMSD noise in an analytical region, and on the absorptivity of the analyte in the same region.

1.4 Data Quality. Data quality shall be determined by executing Protocol pre-test procedures in appendices B to H of the protocol and post-test procedures in appendices I and J of the protocol.

1.4.1 Measurement objectives shall be established by the choice of detection limit (DL_1) and analytical uncertainty (AU_1) for each analyte.

1.4.2 An instrumental configuration shall be selected. An estimate of gas composition shall be made based on previous test data, data from a similar source or information

gathered in a pre-test site survey. Spectral interferants shall be identified using the selected DL_i and AU_i and band areas from reference spectra and interferant spectra. The baseline noise of the system shall be measured in each analytical region to determine the MAU of the instrument configuration for each analyte and interferant (MIU_i).

1.4.3 Data quality for the application shall be determined, in part, by measuring the RMS (root mean square) noise level in each analytical spectral region (appendix C of the Protocol). The RMS noise is defined as the RMSD of the absorbance values in an analytical region from the mean absorbance value in the region.

1.4.4 The MAU is the minimum analyte concentration for which the AU_i can be maintained; if the measured analyte concentration is less than MAU_i , then data quality are unacceptable.

2.0 Summary of Method.

2.1 Principle. References 4 through 7 provide background material on infrared spectroscopy and quantitative analysis. A summary is given in this section.

2.1.1 Infrared absorption spectroscopy is performed by directing an infrared beam through a sample to a detector. The frequency-dependent infrared absorbance of the sample is measured by comparing this detector signal (single beam spectrum) to a signal obtained without a sample in the beam path (background).

2.1.2 Most molecules absorb infrared radiation and the absorbance occurs in a characteristic and reproducible pattern. The infrared spectrum measures fundamental molecular properties and a compound can be identified from its infrared spectrum alone.

2.1.3 Within constraints, there is a linear relationship between infrared absorption and compound concentration. If this frequency dependent relationship (absorptivity) is known (measured), it can be used to determine compound concentration in a sample mixture.

2.1.4 Absorptivity is measured by preparing, in the laboratory, standard samples of compounds at known concentrations and measuring the FTIR "reference spectra" of these standard samples. These "reference spectra" are then used in sample analysis: (1) compounds are detected by matching sample absorbance bands with bands in reference spectra, and (2) concentrations are measured by comparing sample band intensities with reference band intensities.

2.1.5 This method is self-validating provided that the results meet the performance requirement of the QA spike in sections 9.0 and 8.6.2 of this method, and results from a previous method validation study support the use of this method in the application.

2.2 Sampling and Analysis. In extractive sampling a probe assembly and pump are used to extract gas from the exhaust of the affected source and transport the sample to the FTIR gas cell. Typically, the sampling apparatus is similar to that used for single-component continuous emission monitor (CEM) measurements.

2.2.1 The digitized infrared spectrum of the sample in the FTIR gas cell is measured and stored on a computer.

Absorbance band intensities in the spectrum are related to sample concentrations by what is commonly referred to as Beer's Law.

$$A_i = a_i b c_i \quad (1)$$

where:

A_i = absorbance at a given frequency of the i th sample component.

a_i = absorption coefficient (absorptivity) of the i th sample component.

b = path length of the cell.

c_i = concentration of the i th sample component.

2.2.2 Analyte spiking is used for quality assurance (QA). In this procedure (section 8.6.2 of this method) an analyte is spiked into the gas stream at the back end of the sample probe. Analyte concentrations in the spiked samples are compared to analyte concentrations in unspiked samples. Since the concentration of the spike is known, this procedure can be used to determine if the sampling system is removing the spiked analyte(s) from the sample stream.

2.3 Reference Spectra Availability. Reference spectra of over 100 HAPs are available in the EPA FTIR spectral library on the EMTIC (Emission Measurement Technical Information Center) computer bulletin board service and at internet address <http://info.arnold.af.mil/epa/welcome.htm>.

Reference spectra for HAPs, or other analytes, may also be prepared according to section 4.6 of the Protocol.

2.4 Operator Requirements. The FTIR analyst shall be trained in setting up the instrumentation, verifying the instrument is functioning properly, and performing routine maintenance. The analyst must evaluate the initial sample spectra to determine if the sample matrix is consistent with pre-test assumptions and if the instrument configuration is suitable. The analyst must be able to modify the instrument configuration, if necessary.

2.4.1 The spectral analysis shall be supervised by someone familiar with EPA FTIR Protocol procedures.

2.4.2 A technician trained in CEM test methods is qualified to install and operate the sampling system. This includes

installing the probe and heated line assembly, operating the analyte spike system, and performing moisture and flow measurements.

3.0 Definitions.

See appendix A of the Protocol for definitions relating to infrared spectroscopy. Additional definitions are given below.

3.1 Analyte. A compound that this method is used to measure. The term "target analyte" is also used. This method is multi-component and a number of analytes can be targeted for a test.

3.2 Reference Spectrum. Infrared spectrum of an analyte prepared under controlled, documented, and reproducible laboratory conditions according to procedures in section 4.6 of the Protocol. A library of reference spectra is used to measure analytes in gas samples.

3.3 Standard Spectrum. A spectrum that has been prepared from a reference spectrum through a (documented) mathematical operation. A common example is de-resolving of reference spectra to lower-resolution standard spectra (Protocol, appendix K). Standard spectra, prepared by approved, and documented, procedures can be used as reference spectra for analysis.

3.4 Concentration. In this method concentration is expressed as a molar concentration, in ppm-meters, or in (ppm-meters)/K, where K is the absolute temperature (Kelvin). The latter units allow the direct comparison of concentrations from systems using different optical configurations or sampling temperatures.

3.5 Interferant. A compound in the sample matrix whose infrared spectrum overlaps with part of an analyte spectrum. The most accurate analyte measurements are achieved when reference spectra of interferants are used in the quantitative analysis with the analyte reference spectra. The presence of an interferant can increase the analytical uncertainty in the measured analyte concentration.

3.6 Gas Cell. A gas containment cell that can be evacuated. It is equipped with the optical components to pass the infrared beam through the sample to the detector. Important cell features include: path length (or range if variable), temperature range, materials of construction, and total gas volume.

3.7 Sampling System. Equipment used to extract the sample from the test location and transport the sample gas to the FTIR analyzer. This includes sample conditioning systems.

3.8 Sample Analysis. The process of interpreting the infrared spectra to obtain sample analyte concentrations. This process is usually automated using a software routine

employing a classical least squares (cls), partial least squares (pls), or K- or P- matrix method.

3.9 One hundred percent line. A double beam transmittance spectrum obtained by combining two background single beam spectra. Ideally, this line is equal to 100 percent transmittance (or zero absorbance) at every frequency in the spectrum. Practically, a zero absorbance line is used to measure the baseline noise in the spectrum.

3.10 Background Deviation. A deviation from 100 percent transmittance in any region of the 100 percent line. Deviations greater than ± 5 percent in an analytical region are unacceptable (absorbance of 0.021 to -0.022). Such deviations indicate a change in the instrument throughput relative to the background single beam.

3.11 Batch Sampling. A procedure where spectra of discrete, static samples are collected. The gas cell is filled with sample and the cell is isolated. The spectrum is collected. Finally, the cell is evacuated to prepare for the next sample.

3.12 Continuous Sampling. A procedure where spectra are collected while sample gas is flowing through the cell at a measured rate.

3.13 Sampling resolution. The spectral resolution used to collect sample spectra.

3.14 Truncation. Limiting the number of interferogram data points by deleting points farthest from the center burst (zero path difference, ZPD).

3.15 Zero filling. The addition of points to the interferogram. The position of each added point is interpolated from neighboring real data points. Zero filling adds no information to the interferogram, but affects line shapes in the absorbance spectrum (and possibly analytical results).

3.16 Reference CTS. Calibration Transfer Standard spectra that were collected with reference spectra.

3.17 CTS Standard. CTS spectrum produced by applying a de-resolution procedure to a reference CTS.

3.18 Test CTS. CTS spectra collected at the sampling resolution using the same optical configuration as for sample spectra. Test spectra help verify the resolution, temperature and path length of the FTIR system.

3.19 RMSD. Root Mean Square Difference, defined in EPA FTIR Protocol, appendix A.

3.20 Sensitivity. The noise-limited compound-dependent detection limit for the FTIR system configuration. This is estimated by the MAU. It depends on the RMSD in an analytical region of a zero absorbance line.

3.21 Quantitation Limit. The lower limit of detection for the FTIR system configuration in the sample spectra. This

is estimated by mathematically subtracting scaled reference spectra of analytes and interferences from sample spectra, then measuring the RMSD in an analytical region of the subtracted spectrum. Since the noise in subtracted sample spectra may be much greater than in a zero absorbance spectrum, the quantitation limit is generally much higher than the sensitivity. Removing spectral interferences from the sample or improving the spectral subtraction can lower the quantitation limit toward (but not below) the sensitivity.

3.22 Independent Sample. A unique volume of sample gas; there is no mixing of gas between two consecutive independent samples. In continuous sampling two independent samples are separated by at least 5 cell volumes. The interval between independent measurements depends on the cell volume and the sample flow rate (through the cell).

3.23 Measurement. A single spectrum of flue gas contained in the FTIR cell.

3.24 Run. A run consists of a series of measurements. At a minimum a run includes 8 independent measurements spaced over 1 hour.

3.25 Validation. Validation of FTIR measurements is described in sections 13.0 through 13.4 of this method. Validation is used to verify the test procedures for measuring specific analytes at a source. Validation provides proof that the method works under certain test conditions.

3.26 Validation Run. A validation run consists of at least 24 measurements of independent samples. Half of the samples are spiked and half are not spiked. The length of the run is determined by the interval between independent samples.

3.27 Screening. Screening is used when there is little or no available information about a source. The purpose of screening is to determine what analytes are emitted and to obtain information about important sample characteristics such as moisture, temperature, and interferences. Screening results are semi-quantitative (estimated concentrations) or qualitative (identification only). Various optical and sampling configurations may be used. Sample conditioning systems may be evaluated for their effectiveness in removing interferences. It is unnecessary to perform a complete run under any set of sampling conditions. Spiking is not necessary, but spiking can be a useful screening tool for evaluating the sampling system, especially if a reactive or soluble analyte is used for the spike.

3.28 Emissions Test. An FTIR emissions test is performed according specific sampling and analytical procedures. These procedures, for the target analytes and the source, are based on previous screening and validation results.

Emission results are quantitative. A QA spike (sections 8.6.2 and 9.2 of this method) is performed under each set of sampling conditions using a representative analyte. Flow, gas temperature and diluent data are recorded concurrently with the FTIR measurements to provide mass emission rates for detected compounds.

3.29 Surrogate. A surrogate is a compound that is used in a QA spike procedure (section 8.6.2 of this method) to represent other compounds. The chemical and physical properties of a surrogate shall be similar to the compounds it is chosen to represent. Under given sampling conditions, usually a single sampling factor is of primary concern for measuring the target analytes: for example, the surrogate spike results can be representative for analytes that are more reactive, more soluble, have a lower absorptivity, or have a lower vapor pressure than the surrogate itself.

4.0 Interferences.

Interferences are divided into two classifications: analytical and sampling.

4.1 Analytical Interferences. An analytical interference is a spectral feature that complicates (in extreme cases may prevent) the analysis of an analyte. Analytical interferences are classified as background or spectral interference.

4.1.1 Background Interference. This results from a change in throughput relative to the single beam background. It is corrected by collecting a new background and proceeding with the test. In severe instances the cause must be identified and corrected. Potential causes include: (1) deposits on reflective surfaces or transmitting windows, (2) changes in detector sensitivity, (3) a change in the infrared source output, or (4) failure in the instrument electronics. In routine sampling throughput may degrade over several hours. Periodically a new background must be collected, but no other corrective action will be required.

4.1.2 Spectral Interference. This results from the presence of interfering compound(s) (interferant) in the sample. Interferant spectral features overlap analyte spectral features. Any compound with an infrared spectrum, including analytes, can potentially be an interferant. The Protocol measures absorbance band overlap in each analytical region to determine if potential interferants shall be classified as known interferants (FTIR Protocol, section 4.9 and appendix B). Water vapor and CO₂ are common spectral interferants. Both of these compounds have strong infrared spectra and are present in many sample matrices at high concentrations relative to analytes. The extent of interference depends on the (1) interferant concentration,

(2) analyte concentration, and (3) the degree of band overlap. Choosing an alternate analytical region can minimize or avoid the spectral interference. For example, CO_2 interferes with the analysis of the 670 cm^{-1} benzene band. However, benzene can also be measured near 3000 cm^{-1} (with less sensitivity).

4.2 Sampling System Interferences. These prevent analytes from reaching the instrument. The analyte spike procedure is designed to measure sampling system interference, if any.

4.2.1 Temperature. A temperature that is too low causes condensation of analytes or water vapor. The materials of the sampling system and the FTIR gas cell usually set the upper limit of temperature.

4.2.2 Reactive Species. Anything that reacts with analytes. Some analytes, like formaldehyde, polymerize at lower temperatures.

4.2.3 Materials. Poor choice of material for probe, or sampling line may remove some analytes. For example, HF reacts with glass components.

4.2.4 Moisture. In addition to being a spectral interferant, condensed moisture removes soluble compounds.

5.0 Safety.

The hazards of performing this method are those associated with any stack sampling method and the same precautions shall be followed. Many HAPs are suspected carcinogens or present other serious health risks. Exposure to these compounds should be avoided in all circumstances. For instructions on the safe handling of any particular compound, refer to its material safety data sheet. When using analyte standards, always ensure that gases are properly vented and that the gas handling system is leak free. (Always perform a leak check with the system under maximum vacuum and, again, with the system at greater than ambient pressure.) Refer to section 8.2 of this method for leak check procedures. This method does not address all of the potential safety risks associated with its use. Anyone performing this method must follow safety and health practices consistent with applicable legal requirements and with prudent practice for each application.

6.0 Equipment and Supplies.

Note: Mention of trade names or specific products does not constitute endorsement by the Environmental Protection Agency.

The equipment and supplies are based on the schematic of a sampling system shown in Figure 1. Either the batch or continuous sampling procedures may be used with this sampling system. Alternative sampling configurations may also be used, provided that the data quality objectives are met as determined in the post-analysis evaluation. Other

equipment or supplies may be necessary, depending on the design of the sampling system or the specific target analytes.

6.1 Sampling Probe. Glass, stainless steel, or other appropriate material of sufficient length and physical integrity to sustain heating, prevent adsorption of analytes, and to transport analytes to the infrared gas cell. Special materials or configurations may be required in some applications. For instance, high stack sample temperatures may require special steel or cooling the probe. For very high moisture sources it may be desirable to use a dilution probe.

6.2 Particulate Filters. A glass wool plug (optional) inserted at the probe tip (for large particulate removal) and a filter (required) rated for 99 percent removal efficiency at 1-micron (e.g., Balston[®]) connected at the outlet of the heated probe.

6.3 Sampling Line/Heating System. Heated (sufficient to prevent condensation) stainless steel, polytetrafluoroethane, or other material inert to the analytes.

6.4 Gas Distribution Manifold. A heated manifold allowing the operator to control flows of gas standards and samples directly to the FTIR system or through sample conditioning systems. Usually includes heated flow meter, heated valve for selecting and sending sample to the analyzer, and a bypass vent. This is typically constructed of stainless steel tubing and fittings, and high-temperature valves.

6.5 Stainless Steel Tubing. Type 316, appropriate diameter (e.g., 3/8 in.) and length for heated connections. Higher grade stainless may be desirable in some applications.

6.6 Calibration/Analyte Spike Assembly. A three way valve assembly (or equivalent) to introduce analyte or surrogate spikes into the sampling system at the outlet of the probe upstream of the out-of-stack particulate filter and the FTIR analytical system.

6.7 Mass Flow Meter (MFM). These are used for measuring analyte spike flow. The MFM shall be calibrated in the range of 0 to 5 L/min and be accurate to ± 2 percent (or better) of the flow meter span.

6.8 Gas Regulators. Appropriate for individual gas standards.

6.9 Polytetrafluoroethane Tubing. Diameter (e.g., 3/8 in.) and length suitable to connect cylinder regulators to gas standard manifold.

6.10 Sample Pump. A leak-free pump (e.g., KNF[®]), with bypass valve, capable of producing a sample flow rate of at least 10 L/min through 100 ft of sample line. If the pump is positioned upstream of the distribution manifold and FTIR

system, use a heated pump that is constructed from materials non-reactive to the analytes. If the pump is located downstream of the FTIR system, the gas cell sample pressure will be lower than ambient pressure and it must be recorded at regular intervals.

6.11 Gas Sample Manifold. Secondary manifold to control sample flow at the inlet to the FTIR manifold. This is optional, but includes a by-pass vent and heated rotameter.

6.12 Rotameter. A 0 to 20 L/min rotameter. This meter need not be calibrated.

6.13 FTIR Analytical System. Spectrometer and detector, capable of measuring the analytes to the chosen detection limit. The system shall include a personal computer with compatible software allowing automated collection of spectra.

6.14 FTIR Cell Pump. Required for the batch sampling technique, capable of evacuating the FTIR cell volume within 2 minutes. The pumping speed shall allow the operator to obtain 8 sample spectra in 1 hour.

6.15 Absolute Pressure Gauge. Capable of measuring pressure from 0 to 1000 mmHg to within ± 2.5 mmHg (e.g., Baratron).

6.16 Temperature Gauge. Capable of measuring the cell temperature to within $\pm 2^{\circ}\text{C}$.

6.17 Sample Conditioning. One option is a condenser system, which is used for moisture removal. This can be helpful in the measurement of some analytes. Other sample conditioning procedures may be devised for the removal of moisture or other interfering species.

6.17.1 The analyte spike procedure of section 9.2 of this method, the QA spike procedure of section 8.6.2 of this method, and the validation procedure of section 13 of this method demonstrate whether the sample conditioning affects analyte concentrations. Alternatively, measurements can be made with two parallel FTIR systems; one measuring conditioned sample, the other measuring unconditioned sample.

6.17.2 Another option is sample dilution. The dilution factor measurement must be documented and accounted for in the reported concentrations. An alternative to dilution is to lower the sensitivity of the FTIR system by decreasing the cell path length, or to use a short-path cell in conjunction with a long path cell to measure more than one concentration range.

7.0 Reagents and Standards.

7.1 Analyte(s) and Tracer Gas. Obtain a certified gas cylinder mixture containing all of the analyte(s) at concentrations within ± 2 percent of the emission source levels (expressed in ppm-meter/K). If practical, the

analyte standard cylinder shall also contain the tracer gas at a concentration which gives a measurable absorbance at a dilution factor of at least 10:1. Two ppm SF_6 is sufficient for a path length of 22 meters at 250 °F.

7.2 Calibration Transfer Standard(s). Select the calibration transfer standards (CTS) according to section 4.5 of the FTIR Protocol. Obtain a National Institute of Standards and Technology (NIST) traceable gravimetric standard of the CTS (± 2 percent).

7.3 Reference Spectra. Obtain reference spectra for each analyte, interferant, surrogate, CTS, and tracer. If EPA reference spectra are not available, use reference spectra prepared according to procedures in section 4.6 of the EPA FTIR Protocol.

8.0 Sampling and Analysis Procedure.

Three types of testing can be performed: (1) screening, (2) emissions test, and (3) validation. Each is defined in section 3 of this method. Determine the purpose(s) of the FTIR test. Test requirements include: (a) AU_i , DL_i , overall fractional uncertainty, OFU_i , maximum expected concentration (CMAX_i), and t_{AN} for each, (b) potential interferants, (c) sampling system factors, e.g., minimum absolute cell pressure, (P_{min}), FTIR cell volume (V_{SS}), estimated sample absorption pathlength, L_s' , estimated sample pressure, P_s' , T_s' , signal integration time (t_{SS}), minimum instrumental linewidth, MIL, fractional error, and (d) analytical regions, e.g., $m = 1$ to M , lower wavenumber position, FL_m , center wavenumber position, FC_m , and upper wavenumber position, FU_m , plus interferants, upper wavenumber position of the CTS absorption band, FFU_m , lower wavenumber position of the CTS absorption band, FFL_m , wavenumber range FNU to FNL . If necessary, sample and acquire an initial spectrum. From analysis of this preliminary spectrum determine a suitable operational path length. Set up the sampling train as shown in Figure 1 or use an appropriate alternative configuration. Sections 8.1 through 8.11 of this method provide guidance on pre-test calculations in the EPA protocol, sampling and analytical procedures, and post-test protocol calculations.

8.1 Pretest Preparations and Evaluations. Using the procedure in section 4.0 of the FTIR Protocol, determine the optimum sampling system configuration for measuring the target analytes. Use available information to make reasonable assumptions about moisture content and other interferences.

8.1.1 Analytes. Select the required detection limit (DL_i) and the maximum permissible analytical uncertainty (AU_i) for each analyte (labeled from 1 to i). Estimate, if possible, the maximum expected concentration for each analyte, CMAX_i .

The expected measurement range is fixed by DL_i and C_{MAX_i} for each analyte (i).

8.1.2 Potential Interferants. List the potential interferants. This usually includes water vapor and CO_2 , but may also include some analytes and other compounds.

8.1.3. Optical Configuration. Choose an optical configuration that can measure all of the analytes within the absorbance range of .01 to 1.0 (this may require more than one path length). Use Protocol sections 4.3 to 4.8 for guidance in choosing a configuration and measuring CTS.

8.1.4. Fractional Reproducibility Uncertainty (FRU_i). The FRU is determined for each analyte by comparing CTS spectra taken before and after the reference spectra were measured. The EPA para-xylene reference spectra were collected on 10/31/91 and 11/01/91 with corresponding CTS spectra "cts1031a," and "cts1101b." The CTS spectra are used to estimate the reproducibility (FRU) in the system that was used to collect the references. The FRU must be $< AU$. Appendix E of the protocol is used to calculate the FRU from CTS spectra. Figure 2 plots results for 0.25 cm^{-1} CTS spectra in EPA reference library: S_3 (cts1101b - cts1031a), and S_4 [(cts1101b + cts1031a)/2]. The RMSD (SRMS) is calculated in the subtracted baseline, S_3 , in the corresponding CTS region from 850 to 1065 cm^{-1} . The area (BAV) is calculated in the same region of the averaged CTS spectrum, S_4 .

8.1.5 Known Interferants. Use appendix B of the EPA FTIR Protocol.

8.1.6 Calculate the Minimum Analyte Uncertainty, MAU (section 1.3 of this method discusses MAU and protocol appendix D gives the MAU procedure). The MAU for each analyte, i, and each analytical region, m, depends on the RMS noise.

8.1.7 Analytical Program. See FTIR Protocol, section 4.10. Prepare computer program based on the chosen analytical technique. Use as input reference spectra of all target analytes and expected interferants. Reference spectra of additional compounds shall also be included in the program if their presence (even if transient) in the samples is considered possible. The program output shall be in ppm (or ppb) and shall be corrected for differences between the reference path length, L_R , temperature, T_R , and pressure, P_R , and the conditions used for collecting the sample spectra. If sampling is performed at ambient pressure, then any pressure correction is usually small relative to corrections for path length and temperature, and may be neglected.

8.2 Leak-check.

8.2.1 Sampling System. A typical FTIR extractive sampling train is shown in Figure 1. Leak check from the probe tip

to pump outlet as follows: Connect a 0- to 250-mL/min rate meter (rotameter or bubble meter) to the outlet of the pump. Close off the inlet to the probe, and record the leak rate. The leak rate shall be ≤ 200 mL/min.

8.2.2 Analytical System Leak check. Leak check the FTIR cell under vacuum and under pressure (greater than ambient). Leak check connecting tubing and inlet manifold under pressure.

8.2.2.1 For the evacuated sample technique, close the valve to the FTIR cell, and evacuate the absorption cell to the minimum absolute pressure P_{min} . Close the valve to the pump, and determine the change in pressure ΔP_v after 2 minutes.

8.2.2.2 For both the evacuated sample and purging techniques, pressurize the system to about 100 mmHg above atmospheric pressure. Isolate the pump and determine the change in pressure ΔP_p after 2 minutes.

8.2.2.3 Measure the barometric pressure, P_b in mmHg.

8.2.2.4 Determine the percent leak volume $\%V_L$ for the signal integration time t_{ss} and for ΔP_{max} , i.e., the larger of ΔP_v or ΔP_p , as follows:

$$\%V_L = 50 t_{ss} \frac{\Delta P_{max}}{P_{ss}} \quad (2)$$

where 50 = 100% divided by the leak-check time of 2 minutes.

8.2.2.5 Leak volumes in excess of 4 percent of the FTIR system volume V_{ss} are unacceptable.

8.3 Detector Linearity. Once an optical configuration is chosen, use one of the procedures of sections 8.3.1 through 8.3.3 to verify that the detector response is linear. If the detector response is not linear, decrease the aperture, or attenuate the infrared beam. After a change in the instrument configuration perform a linearity check until it is demonstrated that the detector response is linear.

8.3.1 Vary the power incident on the detector by modifying the aperture setting. Measure the background and CTS at three instrument aperture settings: (1) at the aperture setting to be used in the testing, (2) at one half this aperture and (3) at twice the proposed testing aperture. Compare the three CTS spectra. CTS band areas shall agree to within the uncertainty of the cylinder standard and the RMSD noise in the system. If test aperture is the maximum aperture, collect CTS spectrum at maximum aperture, then close the aperture to reduce the IR throughput by half. Collect a second background and CTS at the smaller aperture setting and compare the spectra again.

8.3.2 Use neutral density filters to attenuate the infrared beam. Set up the FTIR system as it will be used in the test measurements. Collect a CTS spectrum. Use a neutral density filter to attenuate the infrared beam (either immediately after the source or the interferometer) to approximately 1/2 its original intensity. Collect a second CTS spectrum. Use another filter to attenuate the infrared beam to approximately 1/4 its original intensity. Collect a third background and CTS spectrum. Compare the CTS spectra. CTS band areas shall agree to within the uncertainty of the cylinder standard and the RMSD noise in the system.

8.3.3 Observe the single beam instrument response in a frequency region where the detector response is known to be zero. Verify that the detector response is "flat" and equal to zero in these regions.

8.4 Data Storage Requirements. All field test spectra shall be stored on a computer disk and a second backup copy must be stored on a separate disk. The stored information includes sample interferograms, processed absorbance spectra, background interferograms, CTS sample interferograms and CTS absorbance spectra. Additionally, documentation of all sample conditions, instrument settings, and test records must be recorded on hard copy or on computer medium. Table 1 gives a sample presentation of documentation.

8.5 Background Spectrum. Evacuate the gas cell to ≤ 5 mmHg, and fill with dry nitrogen gas to ambient pressure (or purge the cell with 10 volumes of dry nitrogen). Verify that no significant amounts of absorbing species (for example water vapor and CO_2) are present. Collect a background spectrum, using a signal averaging period equal to or greater than the averaging period for the sample spectra. Assign a unique file name to the background spectrum. Store two copies of the background interferogram and processed single-beam spectrum on separate computer disks (one copy is the back-up).

8.5.1 Interference Spectra. If possible, collect spectra of known and suspected major interferences using the same optical system that will be used in the field measurements. This can be done on-site or earlier. A number of gases, e.g. CO_2 , SO_2 , CO , NH_3 , are readily available from cylinder gas suppliers.

8.5.2 Water vapor spectra can be prepared by the following procedure. Fill a sample tube with distilled water. Evacuate above the sample and remove dissolved gasses by alternately freezing and thawing the water while evacuating. Allow water vapor into the FTIR cell, then dilute to atmospheric pressure with nitrogen or dry air. If quantitative water spectra are required, follow the

reference spectrum procedure for neat samples (protocol, section 4.6). Often, interference spectra need not be quantitative, but for best results the absorbance must be comparable to the interference absorbance in the sample spectra.

8.6 Pre-Test Calibrations

8.6.1 Calibration Transfer Standard. Evacuate the gas cell to ≤ 5 mmHg absolute pressure, and fill the FTIR cell to atmospheric pressure with the CTS gas. Alternatively, purge the cell with 10 cell volumes of CTS gas. (If purge is used, verify that the CTS concentration in the cell is stable by collecting two spectra 2 minutes apart as the CTS gas continues to flow. If the absorbance in the second spectrum is no greater than in the first, within the uncertainty of the gas standard, then this can be used as the CTS spectrum.) Record the spectrum.

8.6.2 QA Spike. This procedure assumes that the method has been validated for at least some of the target analytes at the source. For emissions testing perform a QA spike. Use a certified standard, if possible, of an analyte, which has been validated at the source. One analyte standard can serve as a QA surrogate for other analytes which are less reactive or less soluble than the standard. Perform the spike procedure of section 9.2 of this method. Record spectra of at least three independent (section 3.22 of this method) spiked samples. Calculate the spiked component of the analyte concentration. If the average spiked concentration is within 0.7 to 1.3 times the expected concentration, then proceed with the testing. If applicable, apply the correction factor from the Method 301 of this appendix validation test (not the result from the QA spike).

8.7 Sampling. If analyte concentrations vary rapidly with time, CEM sampling is preferable using the smallest cell volume, fastest sampling rate and fastest spectra collection rate possible. CEM sampling requires the least operator intervention even without an automated sampling system. For continuous monitoring at one location over long periods, CEM sampling is preferred. Batch sampling and continuous static sampling are used for screening and performing test runs of finite duration. Either technique is preferred for sampling several locations in a matter of days. Batch sampling gives reasonably good time resolution and ensures that each spectrum measures a discreet (and unique) sample volume. Continuous static (and CEM) sampling provide a very stable background over long periods. Like batch sampling, continuous static sampling also ensures that each spectrum measures a unique sample volume. It is essential that the leak check procedure under vacuum (section 8.2 of this

method) is passed if the batch sampling procedure is used. It is essential that the leak check procedure under positive pressure is passed if the continuous static or CEM sampling procedures are used. The sampling techniques are described in sections 8.7.1 through 8.7.2 of this method.

8.7.1 Batch Sampling. Evacuate the absorbance cell to ≤ 5 mmHg absolute pressure. Fill the cell with exhaust gas to ambient pressure, isolate the cell, and record the spectrum. Before taking the next sample, evacuate the cell until no spectral evidence of sample absorption remains. Repeat this procedure to collect eight spectra of separate samples in 1 hour.

8.7.2 Continuous Static Sampling. Purge the FTIR cell with 10 cell volumes of sample gas. Isolate the cell, collect the spectrum of the static sample and record the pressure. Before measuring the next sample, purge the cell with 10 more cell volumes of sample gas.

8.8 Sampling QA and Reporting.

8.8.1 Sample integration times shall be sufficient to achieve the required signal-to-noise ratio. Obtain an absorbance spectrum by filling the cell with N_2 . Measure the RMSD in each analytical region in this absorbance spectrum. Verify that the number of scans used is sufficient to achieve the target MAU.

8.8.2 Assign a unique file name to each spectrum.

8.8.3 Store two copies of sample interferograms and processed spectra on separate computer disks.

8.8.4 For each sample spectrum, document the sampling conditions, the sampling time (while the cell was being filled), the time the spectrum was recorded, the instrumental conditions (path length, temperature, pressure, resolution, signal integration time), and the spectral file name. Keep a hard copy of these data sheets.

8.9 Signal Transmittance. While sampling, monitor the signal transmittance. If signal transmittance (relative to the background) changes by 5 percent or more (absorbance = $-.02$ to $.02$) in any analytical spectral region, obtain a new background spectrum.

8.10 Post-test CTS. After the sampling run, record another CTS spectrum.

8.11 Post-test QA.

8.11.1 Inspect the sample spectra immediately after the run to verify that the gas matrix composition was close to the expected (assumed) gas matrix.

8.11.2 Verify that the sampling and instrumental parameters were appropriate for the conditions encountered. For example, if the moisture is much greater than anticipated,

it may be necessary to use a shorter path length or dilute the sample.

8.11.3 Compare the pre- and post-test CTS spectra. The peak absorbance in pre- and post-test CTS must be ± 5 percent of the mean value. See appendix E of the FTIR Protocol.

9.0 Quality Control.

Use analyte spiking (sections 8.6.2, 9.2 and 13.0 of this method) to verify that the sampling system can transport the analytes from the probe to the FTIR system.

9.1 Spike Materials. Use a certified standard (accurate to ± 2 percent) of the target analyte, if one can be obtained. If a certified standard cannot be obtained, follow the procedures in section 4.6.2.2 of the FTIR Protocol.

9.2 Spiking Procedure. QA spiking (section 8.6.2 of this method) is a calibration procedure used before testing. QA spiking involves following the spike procedure of sections 9.2.1 through 9.2.3 of this method to obtain at least three spiked samples. The analyte concentrations in the spiked samples shall be compared to the expected spike concentration to verify that the sampling system is working properly. Usually, when QA spiking is used, the method has already been validated at a similar source for the analyte in question. The QA spike demonstrates that the validated sampling conditions are being duplicated. If the QA spike fails then the sampling system shall be repaired before testing proceeds. The method validation procedure (section 13.0 of this method) involves a more extensive use of the analyte spike procedure of sections 9.2.1 through 9.2.3 of this method. Spectra of at least 12 independent spiked and 12 independent unspiked samples are recorded. The concentration results are analyzed statistically to determine if there is a systematic bias in the method for measuring a particular analyte. If there is a systematic bias, within the limits allowed by Method 301 of this appendix, then a correction factor shall be applied to the analytical results. If the systematic bias is greater than the allowed limits, this method is not valid and cannot be used.

9.2.1 Introduce the spike/tracer gas at a constant flow rate of ≤ 10 percent of the total sample flow. (Note: Use the rotameter at the end of the sampling train to estimate the required spike/tracer gas flow rate.) Use a flow device, e.g., mass flow meter (± 2 percent), to monitor the spike flow rate. Record the spike flow rate every 10 minutes.

9.2.2 Determine the response time (RT) of the system by continuously collecting spectra of the spiked effluent until the spectrum of the spiked component is constant for 5

minutes. The RT is the interval from the first measurement until the spike becomes constant. Wait for twice the duration of the RT, then collect spectra of two independent spiked gas samples. Duplicate analyses of the spiked concentration shall be within 5 percent of the mean of the two measurements.

9.2.3 Calculate the dilution ratio using the tracer gas as follows:

$$DF = \frac{SF_{6(dlr)}}{SF_{6(sp)}} \quad (3)$$

where:

$$CS = \frac{Spike_{dlr}}{DF} \quad (4)$$

DF	=	Dilution factor of the spike gas; this value shall be ≥ 10 .
$SF_{6(dlr)}$	=	SF_6 (or tracer gas) concentration measured directly in undiluted spike gas.
$SF_{6(sp)}$	=	Diluted SF_6 (or tracer gas) concentration measured in a spiked sample.
$Spike_{dlr}$	=	Concentration of the analyte in the spike standard measured by filling the FTIR cell directly.
CS	=	Expected concentration of the spiked samples.

10.0 Calibration and Standardization.

10.1 Signal-to-Noise Ratio (S/N). The RMSD in the noise must be less than one tenth of the minimum analyte peak absorbance in each analytical region. For example if the minimum peak absorbance is 0.01 at the required DL, then RMSD measured over the entire analytical region must be ≤ 0.001 .

10.2 Absorbance Path length. Verify the absorbance path length by comparing reference CTS spectra to test CTS spectra. See appendix E of the FTIR Protocol.

10.3 Instrument Resolution. Measure the line width of appropriate test CTS band(s) to verify instrument resolution. Alternatively, compare CTS spectra to a reference CTS spectrum, if available, measured at the nominal resolution.

10.4 Apodization Function. In transforming the sample interferograms to absorbance spectra use the same apodization function that was used in transforming the reference spectra.

10.5 FTIR Cell Volume. Evacuate the cell to ≤ 5 mmHg. Measure the initial absolute temperature (T_i) and absolute pressure (P_i). Connect a wet test meter (or a calibrated dry gas meter), and slowly draw room air into the cell. Measure the meter volume (V_m), meter absolute temperature (T_m), and meter absolute pressure (P_m); and the cell final absolute temperature (T_f) and absolute pressure (P_f). Calculate the FTIR cell volume V_{ss} , including that of the connecting tubing, as follows:

$$V_{ss} = \frac{V_m \frac{P_m}{T_m}}{\left[\frac{P_f}{T_f} - \frac{P_i}{T_i} \right]} \quad (5)$$

11.0 Data Analysis and Calculations.

Analyte concentrations shall be measured using reference spectra from the EPA FTIR spectral library. When EPA library spectra are not available, the procedures in section 4.6 of the Protocol shall be followed to prepare reference spectra of all the target analytes.

11.1 Spectral De-resolution. Reference spectra can be converted to lower resolution standard spectra (section 3.3 of this method) by truncating the original reference sample and background interferograms. Appendix K of the FTIR Protocol gives specific deresolution procedures. Deresolved spectra shall be transformed using the same apodization function and level of zero filling as the sample spectra. Additionally, pre-test FTIR protocol calculations (e.g., FRU, MAU, FCU) shall be performed using the de-resolved standard spectra.

11.2 Data Analysis. Various analytical programs are available for relating sample absorbance to a concentration standard. Calculated concentrations shall be verified by analyzing residual baselines after mathematically subtracting scaled reference spectra from the sample spectra. A full description of the data analysis and calculations is contained in the FTIR Protocol (sections

4.0, 5.0, 6.0 and appendices). Correct the calculated concentrations in the sample spectra for differences in absorption path length and temperature between the reference and sample spectra using equation 6,

$$C_{corr} = \left(\frac{L_r}{L_s} \right) \left(\frac{T_s}{T_r} \right) C_{calc} \quad (6)$$

where:

C_{corr} = Concentration, corrected for path length.

C_{calc} = Concentration, initial calculation (output of the analytical program designed for the compound).

L_r = Reference spectra path length.

L_s = Sample spectra path length.

T_s = Absolute temperature of the sample gas, K.

T_r = Absolute gas temperature of reference spectra, K.

12.0 Method Performance.

12.1 Spectral Quality. Refer to the FTIR Protocol appendices for analytical requirements, evaluation of data quality, and analysis of uncertainty.

12.2 Sampling QA/QC. The analyte spike procedure of section 9 of this method, the QA spike of section 8.6.2 of this method, and the validation procedure of section 13 of this method are used to evaluate the performance of the sampling system and to quantify sampling system effects, if any, on the measured concentrations. This method is self-validating provided that the results meet the performance

requirement of the QA spike in sections 9.0 and 8.6.2 of this method and results from a previous method validation study support the use of this method in the application. Several factors can contribute to uncertainty in the measurement of spiked samples. Factors which can be controlled to provide better accuracy in the spiking procedure are listed in sections 12.2.1 through 12.2.4 of this method.

12.2.1 Flow meter. An accurate mass flow meter is accurate to ± 1 percent of its span. If a flow of 1 L/min is monitored with such a MFM, which is calibrated in the range of 0-5 L/min, the flow measurement has an uncertainty of 5 percent. This may be improved by re-calibrating the meter at the specific flow rate to be used.

12.2.2 Calibration gas. Usually the calibration standard is certified to within ± 2 percent. With reactive analytes, such as HCl, the certified accuracy in a commercially available standard may be no better than ± 5 percent.

12.2.3 Temperature. Temperature measurements of the cell shall be quite accurate. If practical, it is preferable to measure sample temperature directly, by inserting a thermocouple into the cell chamber instead of monitoring the cell outer wall temperature.

12.2.4 Pressure. Accuracy depends on the accuracy of the barometer, but fluctuations in pressure throughout a day may be as much as 2.5 percent due to weather variations.

13.0 Method Validation Procedure.

This validation procedure, which is based on EPA Method 301 (40 CFR part 63, appendix A), may be used to validate this method for the analytes in a gas matrix. Validation at one source may also apply to another type of source, if it can be shown that the exhaust gas characteristics are similar at both sources.

13.1 Section 5.3 of Method 301 (40 CFR part 63, appendix A), the Analyte Spike procedure, is used with these modifications. The statistical analysis of the results follows section 6.3 of EPA Method 301. Section 3 of this method defines terms that are not defined in Method 301.

13.1.1 The analyte spike is performed dynamically. This means the spike flow is continuous and constant as spiked samples are measured.

13.1.2 The spike gas is introduced at the back of the sample probe.

13.1.3 Spiked effluent is carried through all sampling components downstream of the probe.

13.1.4 A single FTIR system (or more) may be used to collect and analyze spectra (not quadruplicate integrated sampling trains).

13.1.5 All of the validation measurements are performed sequentially in a single "run" (section 3.26 of this method).

13.1.6 The measurements analyzed statistically are each independent (section 3.22 of this method).

13.1.7 A validation data set can consist of more than 12 spiked and 12 unspiked measurements.

13.2 Batch Sampling. The procedure in sections 13.2.1 through 13.2.2 may be used for stable processes. If process emissions are highly variable, the procedure in section 13.2.3 shall be used.

13.2.1 With a single FTIR instrument and sampling system, begin by collecting spectra of two unspiked samples.

Introduce the spike flow into the sampling system and allow 10 cell volumes to purge the sampling system and FTIR cell. Collect spectra of two spiked samples. Turn off the spike and allow 10 cell volumes of unspiked sample to purge the FTIR cell. Repeat this procedure until the 24 (or more) samples are collected.

13.2.2 In batch sampling, collect spectra of 24 distinct samples. (Each distinct sample consists of filling the cell to ambient pressure after the cell has been evacuated.)

13.2.3 Alternatively, a separate probe assembly, line, and sample pump can be used for spiked sample. Verify and document that sampling conditions are the same in both the

spiked and the unspiked sampling systems. This can be done by wrapping both sample lines in the same heated bundle. Keep the same flow rate in both sample lines. Measure samples in sequence in pairs. After two spiked samples are measured, evacuate the FTIR cell, and turn the manifold valve so that spiked sample flows to the FTIR cell. Allow the connecting line from the manifold to the FTIR cell to purge thoroughly (the time depends on the line length and flow rate). Collect a pair of spiked samples. Repeat the procedure until at least 24 measurements are completed.

13.3 Simultaneous Measurements With Two FTIR Systems. If unspiked effluent concentrations of the target analyte(s) vary significantly with time, it may be desirable to perform synchronized measurements of spiked and unspiked sample. Use two FTIR systems, each with its own cell and sampling system to perform simultaneous spiked and unspiked measurements. The optical configurations shall be similar, if possible. The sampling configurations shall be the same. One sampling system and FTIR analyzer shall be used to measure spiked effluent. The other sampling system and FTIR analyzer shall be used to measure unspiked flue gas. Both systems shall use the same sampling procedure (i.e., batch or continuous).

13.3.1 If batch sampling is used, synchronize the cell evacuation, cell filling, and collection of spectra. Fill both cells at the same rate (in cell volumes per unit time).

13.3.2 If continuous sampling is used, adjust the sample flow through each gas cell so that the same number of cell volumes pass through each cell in a given time (i.e. $TC_1 = TC_2$).

13.4 Statistical Treatment. The statistical procedure of EPA Method 301 of this appendix, section 6.3 is used to evaluate the bias and precision. For FTIR testing a validation "run" is defined as spectra of 24 independent samples, 12 of which are spiked with the analyte(s) and 12 of which are not spiked.

13.4.1 Bias. Determine the bias (defined by EPA Method 301 of this appendix, section 6.3.2) using equation 7:

$$B = S_s - M_u - CS \quad (7)$$

where:

B = Bias at spike level.

S_s = Mean concentration of the analyte spiked samples.

M_u = Mean concentration of the unspiked samples.

CS = Expected concentration of the spiked samples.

13.4.2 Correction Factor. Use section 6.3.2.2 of Method 301 of this appendix to evaluate the statistical significance of the bias. If it is determined that the bias

is significant, then use section 6.3.3 of Method 301 to calculate a correction factor (CF). Analytical results of the test method are multiplied by the correction factor, if $0.7 \leq CF \leq 1.3$. If it is determined that the bias is significant and $CF > \pm 30$ percent, then the test method is considered to "not valid."

13.4.3 If measurements do not pass validation, evaluate the sampling system, instrument configuration, and analytical system to determine if improper set-up or a malfunction was the cause. If so, repair the system and repeat the validation.

14.0 Pollution Prevention.

The extracted sample gas is vented outside the enclosure containing the FTIR system and gas manifold after the analysis. In typical method applications the vented sample volume is a small fraction of the source volumetric flow and its composition is identical to that emitted from the source. When analyte spiking is used, spiked pollutants are vented with the extracted sample gas. Approximately 1.6×10^{-4} to 3.2×10^{-4} lbs of a single HAP may be vented to the atmosphere in a typical validation run of 3 hours. (This assumes a molar mass of 50 to 100 g, spike rate of 1.0 L/min, and a standard concentration of 100 ppm). Minimize emissions by keeping the spike flow off when not in use.

15.0 Waste Management.

Small volumes of laboratory gas standards can be vented through a laboratory hood. Neat samples must be packed and disposed according to applicable regulations. Surplus materials may be returned to supplier for disposal.

16.0 References.

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2. "FTIR Method Validation at a Coal-Fired Boiler". Prepared for U.S. Environmental Protection Agency, Research Triangle Park, NC. Publication No.: EPA-454/R95-004, NTIS No.: PB95-193199. July, 1993.
3. "Method 301 - Field Validation of Pollutant Measurement Methods from Various Waste Media," **40 CFR part 63, appendix A.**
4. "Molecular Vibrations; The Theory of Infrared and Raman Vibrational Spectra," E. Bright Wilson, J. C. Decius, and P. C. Cross, Dover Publications, Inc., 1980. For a less intensive treatment of molecular rotational-vibrational spectra see, for example, "Physical Chemistry," G. M. Barrow, chapters 12, 13, and 14, McGraw Hill, Inc., 1979.

5. "Fourier Transform Infrared Spectrometry," Peter R. Griffiths and James de Haseth, **Chemical Analysis**, **83**, 16-25, (1986), P. J. Elving, J. D. Winefordner and I. M. Kolthoff (ed.), John Wiley and Sons.
6. "Computer-Assisted Quantitative Infrared Spectroscopy," Gregory L. McClure (ed.), **ASTM Special Publication 934** (ASTM), 1987.
7. "Multivariate Least-Squares Methods Applied to the Quantitative Spectral Analysis of Multicomponent Mixtures," **Applied Spectroscopy**, **39**(10), 73-84, 1985.

Table 1. EXAMPLE PRESENTATION OF SAMPLING DOCUMENTATION.

Sample Time	Spectrum File Name	Background File Name	Sample conditioning	Process condition

Sample Time	Spectrum File	Interferogram	Resolution	Scans	Apodization	Gain	CTS Spectrum

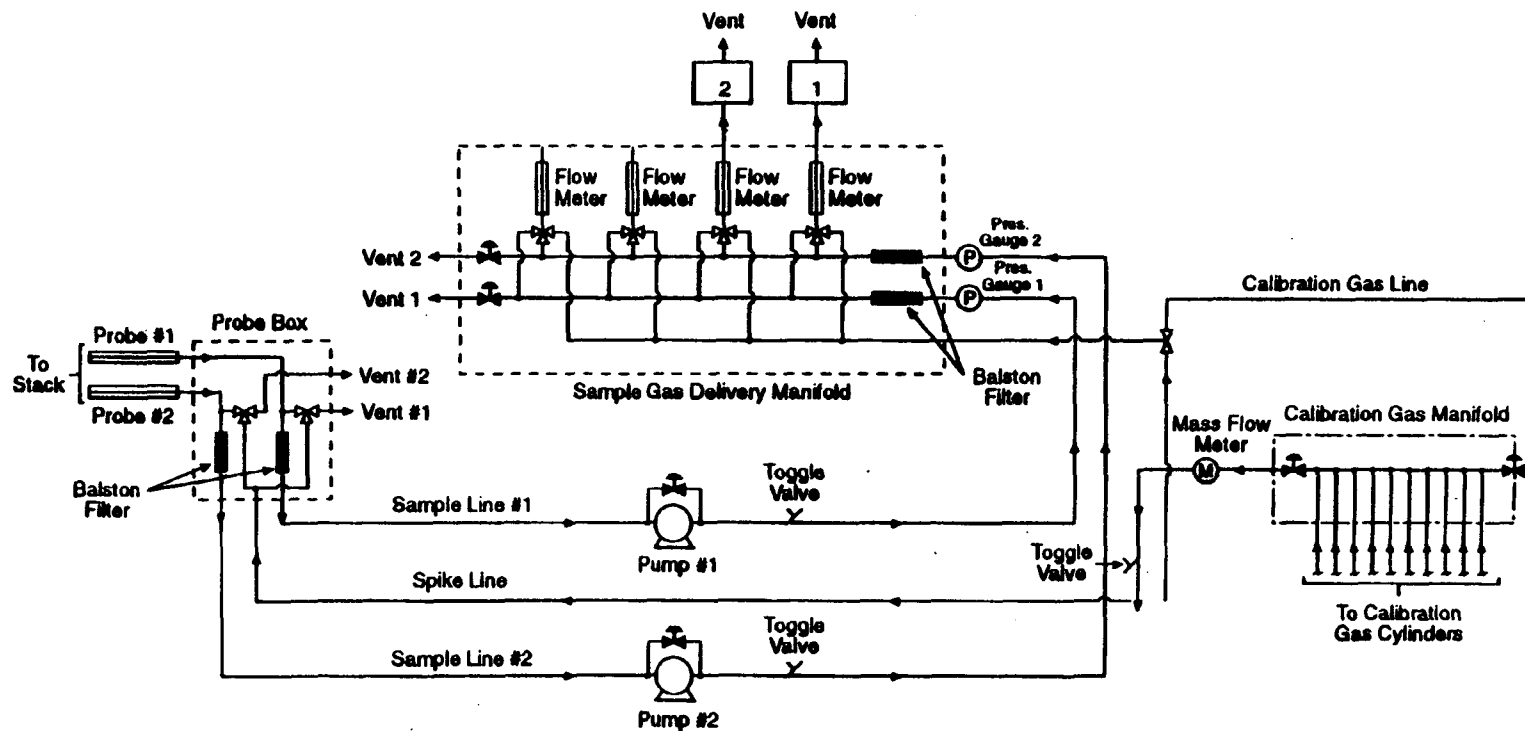


Figure 1. Extractive FTIR sampling system.

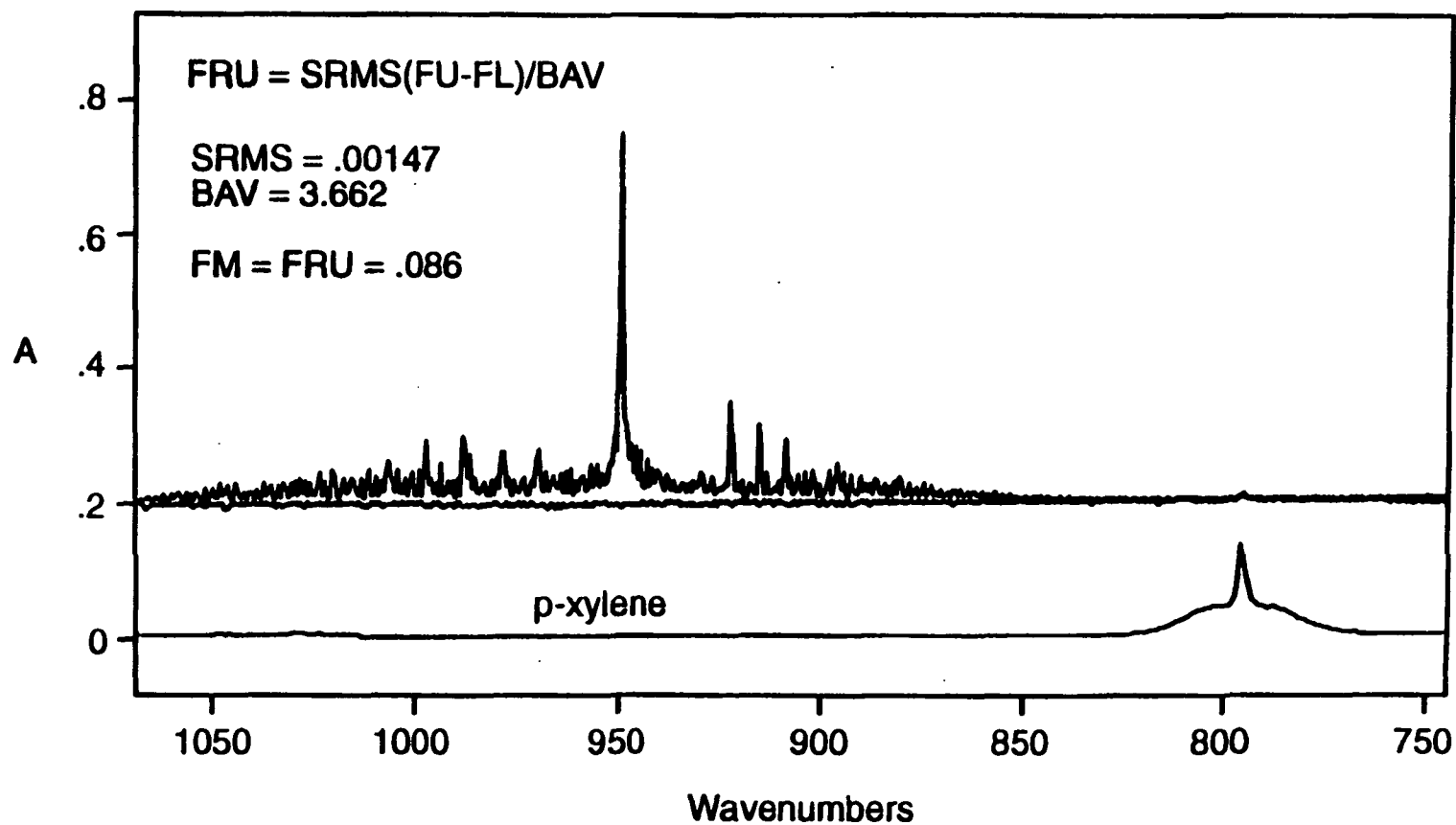


Figure 2. Fractional Reproducibility. Top: average of cts1031a and cts1101b. Bottom: Reference spectrum of p-xylene.

**PROTOCOL FOR THE USE OF EXTRACTIVE FOURIER TRANSFORM
INFRARED (FTIR) SPECTROMETRY FOR THE ANALYSES OF GASEOUS
EMISSIONS FROM STATIONARY SOURCES**

INTRODUCTION

The purpose of this document is to set general guidelines for the use of modern FTIR spectroscopic methods for the analysis of gas samples extracted from the effluent of stationary emission sources. This document outlines techniques for developing and evaluating such methods and sets basic requirements for reporting and quality assurance procedures.

1.0 NOMENCLATURE

1.1 Appendix A lists definitions of the symbols and terms used in this Protocol, many of which have been taken directly from American Society for Testing and Materials (ASTM) publication E 131-90a, entitled "Terminology Relating to Molecular Spectroscopy."

1.2 Except in the case of background spectra or where otherwise noted, the term "spectrum" refers to a double-beam spectrum in units of absorbance vs. wavenumber (cm^{-1}).

1.3 The term "Study" in this document refers to a publication that has been subjected to EPA- or peer-review.

2.0 APPLICABILITY AND ANALYTICAL PRINCIPLE

2.1 Applicability. This Protocol applies to the determination of compound-specific concentrations in single- and multiple-component gas phase samples using double-beam absorption spectroscopy in the mid-infrared band. It does not specifically address other FTIR applications, such as single-beam spectroscopy, analysis of open-path (non-enclosed) samples, and continuous measurement techniques. If multiple spectrometers, absorption cells, or instrumental linewidths are used in such analyses, each distinct operational configuration of the system must be evaluated separately according to this Protocol.

2.2 Analytical Principle.

2.2.1 In the mid-infrared band, most molecules exhibit characteristic gas phase absorption spectra that may be recorded by FTIR systems. Such systems consist of a source of mid-infrared radiation, an interferometer, an enclosed sample cell of known absorption pathlength, an infrared detector, optical elements for the transfer of infrared radiation between components, and gas flow control and measurement components. Adjunct and integral computer systems are used for controlling the instrument, processing the signal, and for performing both Fourier transforms and quantitative analyses of spectral data.

2.2.2 The absorption spectra of pure gases and of mixtures of gases are described by a linear absorbance theory referred to as Beer's Law. Using this law, modern FTIR systems use computerized analytical programs to quantify compounds by comparing the absorption spectra of known (reference) gas samples to the absorption spectrum of the sample gas. Some standard mathematical techniques used for comparisons are classical least squares, inverse least squares, cross-correlation, factor analysis, and partial least squares. Reference A describes several of these techniques, as well as additional techniques, such as differentiation methods, linear baseline corrections, and non-linear absorbance corrections.

3.0 GENERAL PRINCIPLES OF PROTOCOL REQUIREMENTS

The characteristics that distinguish FTIR systems from gas analyzers used in instrumental gas analysis methods (e.g., EPA Methods 6C and 7E) are: (1) Computers are necessary to obtain and analyze data; (2) chemical concentrations can be quantified using previously recorded infrared reference spectra; and (3) analytical assumptions and results, including possible effects of interfering compounds, can be evaluated after the quantitative analysis. The following general principles and requirements of this Protocol are based on these characteristics.

3.1 Verifiability and Reproducibility of Results. Store all data and document data analysis techniques sufficient to allow an independent agent to reproduce the analytical results from the raw interferometric data.

3.2 Transfer of Reference Spectra. To determine whether reference spectra recorded under one set of conditions (e.g., optical bench, instrumental linewidth, absorption pathlength, detector performance, pressure, and temperature) can be used to analyze sample spectra taken under a different set of conditions, quantitatively compare "calibration transfer standards" (CTS) and reference spectra as described in this Protocol. (Note: The CTS may, but need not, include analytes of interest). To effect this, record the absorption spectra of the CTS (a) immediately before and immediately after recording reference spectra and (b) immediately after recording sample spectra.

3.3 Evaluation of FTIR Analyses. The applicability, accuracy, and precision of FTIR measurements are influenced by a number of interrelated factors, which may be divided into two classes:

3.3.1 Sample-Independent Factors. Examples are system configuration and performance (e.g., detector sensitivity and infrared source output), quality and applicability of reference absorption spectra, and type of mathematical analyses of the spectra. These factors define the fundamental limitations of FTIR measurements for a given system configuration. These limitations may be estimated from evaluations of the system before samples are available. For example, the detection limit for the absorbing compound under a given set of conditions may be

estimated from the system noise level and the strength of a particular absorption band. Similarly, the accuracy of measurements may be estimated from the analysis of the reference spectra.

3.3.2 Sample-Dependent Factors. Examples are spectral interferants (e.g., water vapor and CO_2) or the overlap of spectral features of different compounds and contamination deposits on reflective surfaces or transmitting windows. To maximize the effectiveness of the mathematical techniques used in spectral analysis, identification of interferants (a standard initial step) and analysis of samples (includes effects of other analytical errors) are necessary. Thus, the Protocol requires post-analysis calculation of measurement concentration uncertainties for the detection of these potential sources of measurement error.

4.0 PRE-TEST PREPARATIONS AND EVALUATIONS

Before testing, demonstrate the suitability of FTIR spectrometry for the desired application according to the procedures of this section.

4.1 Identify Test Requirements. Identify and record the test requirements described below in 4.1.1 through 4.1.5. These values set the desired or required goals of the proposed analysis; the description of methods for determining whether these goals are actually met during the analysis comprises the majority of this Protocol.

4.1.1 Analytes (specific chemical species) of interest. Label the analytes from $i = 1$ to I .

4.1.2 Analytical uncertainty limit (AU_i). The AU_i is the maximum permissible fractional uncertainty of analysis for the i^{th} analyte concentration, expressed as a fraction of the analyte concentration in the sample.

4.1.3 Required detection limit for each analyte (DL_i , ppm). The detection limit is the lowest concentration of an analyte for which its overall fractional uncertainty (OFU_i) is required to be less than its analytical uncertainty limit (AU_i).

4.1.4 Maximum expected concentration of each analyte (CMAX_i , ppm).

4.2 Identify Potential Interferants. Considering the chemistry of the process or results of previous Studies, identify potential interferants, i.e., the major effluent constituents and any relatively minor effluent constituents that possess either strong absorption characteristics or strong structural similarities to any analyte of interest. Label them 1 through N_j , where the subscript "j" pertains to potential interferants. Estimate the concentrations of these compounds in the effluent (CPOT_j , ppm).

4.3 Select and Evaluate the Sampling System. Considering the source, e.g., temperature and pressure profiles, moisture content, analyte characteristics, and particulate concentration), select the equipment for extracting gas samples. Recommended are a particulate filter, heating system to maintain sample temperature above the dew point for all sample constituents at all points within the sampling system (including the filter), and sample conditioning system (e.g., coolers, water-permeable membranes that remove water or other compounds from the sample, and dilution devices) to remove spectral interferants or to protect the sampling and analytical components. Determine the minimum absolute sample system pressure (P_{\min} , mmHg) and the infrared absorption cell volume (V_{ss} , liter). Select the techniques and/or equipment for the measurement of sample pressures and temperatures.

4.4 Select Spectroscopic System. Select a spectroscopic configuration for the application. Approximate the absorption pathlength (L_s , meter), sample pressure (P_s , kPa), absolute sample temperature T_s , and signal integration period (t_{ss} , seconds) for the analysis. Specify the nominal minimum instrumental linewidth (MIL) of the system. Verify that the fractional error at the approximate values P_s and T_s is less than one half the smallest value AU_i (see Section 4.1.2).

4.5 Select Calibration Transfer Standards (CTS's). Select CTS's that meet the criteria listed in Sections 4.5.1, 4.5.2, and 4.5.3.

Note: It may be necessary to choose preliminary analytical regions (see Section 4.7), identify the minimum analyte linewidths, or estimate the system noise level (see Section 4.12) before selecting the CTS. More than one compound may be needed to meet the criteria; if so, obtain separate cylinders for each compound.

4.5.1 The central wavenumber position of each analytical region lies within 25 percent of the wavenumber position of at least one CTS absorption band.

4.5.2 The absorption bands in 4.5.1 exhibit peak absorbances greater than ten times the value RMS_{EST} (see Section 4.12) but less than 1.5 absorbance units.

4.5.3 At least one absorption CTS band within the operating range of the FTIR instrument has an instrument-independent linewidth no greater than the narrowest analyte absorption band; perform and document measurements or cite Studies to determine analyte and CTS compound linewidths.

4.5.4 For each analytical region, specify the upper and lower wavenumber positions (FFU_m and FFL_m , respectively) that bracket the CTS absorption band or bands for the associated analytical region. Specify the wavenumber range, FNU to FNL, containing the absorption band that meets the criterion of Section 4.5.3.

4.5.5 Associate, whenever possible, a single set of CTS gas cylinders with a set of reference spectra. Replacement CTS gas cylinders shall contain the same compounds at concentrations within 5 percent of that of the original CTS cylinders; the entire absorption spectra (not individual spectral segments) of the replacement gas shall be scaled by a factor between 0.95 and 1.05 to match the original CTS spectra.

4.6 Prepare Reference Spectra.

Note: Reference spectra are available in a permanent soft copy from the EPA spectral library on the EMTIC (Emission Measurement Technical Information Center) computer bulletin board; they may be used if applicable.

4.6.1 Select the reference absorption pathlength (L_R) of the cell.

4.6.2 Obtain or prepare a set of chemical standards for each analyte, potential and known spectral interferants, and CTS. Select the concentrations of the chemical standards to correspond to the top of the desired range.

4.6.2.1 Commercially-Prepared Chemical Standards. Chemical standards for many compounds may be obtained from independent sources, such as a specialty gas manufacturer, chemical company, or commercial laboratory. These standards (accurate to within ± 2 percent) shall be prepared according to EPA Protocol 1 (see Reference D) or shall be traceable to NIST standards. Obtain from the supplier an estimate of the stability of the analyte concentration; obtain and follow all the supplier's recommendations for recertifying the analyte concentration.

4.6.2.2 Self-Prepared Chemical Standards. Chemical standards may be prepared as follows: Dilute certified commercially prepared chemical gases or pure analytes with ultra-pure carrier (UPC) grade nitrogen according to the barometric and volumetric techniques generally described in Reference A, Section A4.6.

4.6.3 Record a set of the absorption spectra of the CTS (R_1), then a set of the reference spectra at two or more concentrations in duplicate over the desired range (the top of the range must be less than 10 times that of the bottom), followed by a second set of CTS spectra (R_2). (If self-prepared standards are used, see Section 4.6.5 before disposing of any of the standards.) The maximum accepted standard concentration-pathlength product (ASCPP) for each compound shall be higher than the maximum estimated concentration-pathlength products for both analytes and known interferants in the effluent gas. For each analyte, the minimum ASCPP shall be no greater than ten times the concentration-pathlength product of that analyte at its required detection limit.

4.6.4 Permanently store the background and interferograms in digitized form. Document details of the mathematical process for generating the spectra from these interferograms. Record the

sample pressure (P_R), sample temperature (T_R), reference absorption pathlength (L_R), and interferogram signal integration period (t_{SR}). Signal integration periods for the background interferograms shall be $\geq t_{SR}$. Values of P_R , L_R , and t_{SR} shall not deviate by more than ± 1 percent from the time of recording {R1} to that of recording {R2}.

4.6.5 If self-prepared chemical standards are employed and spectra of only two concentrations are recorded for one or more compounds, verify the accuracy of the dilution technique by analyzing the prepared standards for those compounds with a secondary (non-FTIR) technique as follows:

4.6.5.1 Record the response of the secondary technique to each of the four standards prepared.

4.6.5.2 Perform a linear regression of the response values (dependant variable) versus the accepted standard concentration (ASC) values (independent variable), with the regression constrained to pass through the zero-response, zero ASC point.

4.6.5.3 Calculate the average fractional difference between the actual response values and the regression-predicted values (those calculated from the regression line using the four ASC values as the independent variable).

4.6.5.4 If the average fractional difference value calculated in Section 4.6.5.3 is larger for any compound than the corresponding AU_i , the dilution technique is not sufficiently accurate and the reference spectra prepared are not valid for the analysis.

4.7 Select Analytical Regions. Using the general considerations in Section 7 of Reference A and the spectral characteristics of the analytes and interferants, select the analytical regions for the application. Label them $m = 1$ to M . Specify the lower, center and upper wavenumber positions of each analytical region (FL_m , FC_m , and FU_m , respectively). Specify the analytes and interferants which exhibit absorption in each region.

4.8 Determine Fractional Reproducibility Uncertainties. Using Appendix E, calculate the fractional reproducibility uncertainty for each analyte (FRU_i) from a comparison of {R1} and {R2}. If $FRU_i > AU_i$ for any analyte, the reference spectra generated in Section 4.6 are not valid for the application.

4.9 Identify Known Interferants. Using Appendix B, determine which potential interferant affects the analyte concentration determinations. If it does, relabel the potential interferant as "known" interferant, and designate these compounds from $k = 1$ to K . Appendix B also provides criteria for determining whether the selected analytical regions are suitable.

4.10 Prepare Computerized Analytical Programs.

4.10.1 Choose or devise mathematical techniques (e.g., classical least squares, inverse least squares, cross-correlation, and factor analysis) based on Equation 4 of Reference A that are appropriate for analyzing spectral data by comparison with reference spectra.

4.10.2 Following the general recommendations of Reference A, prepare a computer program or set of programs that analyzes all the analytes and known interferants, based on the selected analytical regions (4.7) and the prepared reference spectra (4.6). Specify the baseline correction technique (e.g., determining the slope and intercept of a linear baseline contribution in each analytical region) for each analytical region, including all relevant wavenumber positions.

4.10.3 Use programs that provide as output [at the reference absorption pathlength (L_R), reference gas temperature (T_R), and reference gas pressure (P_R)] the analyte concentrations, the known interferant concentrations, and the baseline slope and intercept values. If the sample absorption pathlength (L_S), sample gas temperature (T_S) or sample gas pressure (P_S) during the actual sample analyses differ from L_R , T_R , and P_R , use a program or set of programs that applies multiplicative corrections to the derived concentrations to account for these variations, and that provides as output both the corrected and uncorrected values. Include in the report of the analysis (see Section 7.0) the details of any transformations applied to the original reference spectra (e.g., differentiation), in such a fashion that all analytical results may be verified by an independent agent from the reference spectra and data spectra alone.

4.11 Determine the Fractional Calibration Uncertainty. Calculate the fractional calibration uncertainty for each analyte (FCU_i) according to Appendix F, and compare these values to the fractional uncertainty limits (AU_i ; see Section 4.1). If $FCU_i > AU_i$, either the reference spectra or analytical programs for that analyte are unsuitable.

4.12 Verify System Configuration Suitability. Using Appendix C, measure or obtain estimates of the noise level (RMS_{EST} , absorbance) of the FTIR system; alternatively, construct the complete spectrometer system and determine the values RMS_{sm} using Appendix G. Estimate the minimum measurement uncertainty for each analyte (MAU_i , ppm) and known interferant (MIU_k , ppm) using Appendix D. Verify that (a) $MAU_i < (AU_i)(DL_i)$, $FRU_i < AU_i$, and $FCU_i < AU_i$ for each analyte and that (b) the CTS chosen meets the requirements listed in Section 4.5.

5.0 SAMPLING AND ANALYSIS PROCEDURE

5.1 Analysis System Assembly and Leak-Test. Assemble the analysis system. Allow sufficient time for all system components to reach the desired temperature. Then determine the leak-rate (L_R) and leak volume (V_L), where $V_L = L_R t_{ss}$. Leak volumes shall be ≤ 4 percent of V_{ss} .

5.2 Verify Instrumental Performance. Measure the noise level of the system in each analytical region using the procedure of Appendix G. If any noise level is higher than that estimated for the system in Section 4.12, repeat the calculations of Appendix D and verify that the requirements of Section 4.12 are met; if they are not, adjust or repair the instrument and repeat this section.

5.3 Determine the Sample Absorption Pathlength. Record a background spectrum. Then, fill the absorption cell with CTS at the pressure P_R and record a set of CTS spectra $\{R3\}$. Store the background and unscaled CTS single beam interferograms and spectra. Using Appendix H, calculate the sample absorption pathlength (L_s) for each analytical region. The values L_s shall not differ from the approximated sample pathlength L_s' (see Section 4.4) by more than 5 percent.

5.4 Record Sample Spectrum. Connect the sample line to the source. Either evacuate the absorption cell to an absolute pressure below 5 mmHg before extracting a sample from the effluent stream into the absorption cell, or pump at least ten cell volumes of sample through the cell before obtaining a sample. Record the sample pressure P_s . Generate the absorbance spectrum of the sample. Store the background and sample single beam interferograms, and document the process by which the absorbance spectra are generated from these data. (If necessary, apply the spectral transformations developed in Section 5.6.2). The resulting sample spectrum is referred to below as S_s .

Note: Multiple sample spectra may be recorded according to the procedures of Section 5.4 before performing Sections 5.5 and 5.6.

5.5 Quantify Analyte Concentrations. Calculate the unscaled analyte concentrations RUA_i and unscaled interferant concentrations RUI_k using the programs developed in Section 4. To correct for pathlength and pressure variations between the reference and sample spectra, calculate the scaling factor $R_{LPS} = (L_R P_R T_s) / (L_s P_s T_R)$. Calculate the final analyte and interferant concentrations $RSA_i = R_{LPS} RUA_i$ and $RSI_k = R_{LPS} RUI_k$.

5.6 Determine Fractional Analysis Uncertainty. Fill the absorption cell with CTS at the pressure P_s . Record a set of CTS spectra $\{R4\}$. Store the background and CTS single beam interferograms. Using Appendix H, calculate the fractional analysis uncertainty (FAU) for each analytical region. If the FAU indicated for any analytical region is larger than the required accuracy requirements determined in Section 4.1, then comparisons to previously recorded reference spectra are invalid in that analytical region, and the analyst shall perform one or both of the following procedures:

5.6.1 Perform instrumental checks and adjust the instrument to restore its performance to acceptable levels. If adjustments are made, repeat Sections 5.3, 5.4 (except for the recording of a sample spectrum), and 5.5 to demonstrate that acceptable uncertainties are obtained in all analytical regions.

5.6.2 Apply appropriate mathematical transformations (e.g., frequency shifting, zero-filling, apodization, smoothing) to the spectra (or to the interferograms upon which the spectra are based) generated during the performance of the procedures of Section 5.3. Document these transformations and their reproducibility. Do not apply multiplicative scaling of the spectra, or any set of transformations that is mathematically equivalent to multiplicative scaling. Different transformations may be applied to different analytical regions. Frequency shifts shall be smaller than one-half the minimum instrumental linewidth, and must be applied to all spectral data points in an analytical region. The mathematical transformations may be retained for the analysis if they are also applied to the appropriate analytical regions of all sample spectra recorded, and if all original sample spectra are digitally stored. Repeat Sections 5.3, 5.4 (except the recording of a sample spectrum), and 5.5 to demonstrate that these transformations lead to acceptable calculated concentration uncertainties in all analytical regions.

6.0 POST-ANALYSIS EVALUATIONS

Estimate the overall accuracy of the analyses performed in Section 5 as follows:

6.1 Qualitatively Confirm the Assumed Matrix. Examine each analytical region of the sample spectrum for spectral evidence of unexpected or unidentified interferants. If found, identify the interfering compounds (see Reference C for guidance) and add them to the list of known interferants. Repeat the procedures of Section 4 to include the interferants in the uncertainty calculations and analysis procedures. Verify that the MAU and FCU values do not increase beyond acceptable levels for the application requirements. Re-calculate the analyte concentrations (Section 5.5) in the affected analytical regions.

6.2 Quantitatively Evaluate Fractional Model Uncertainty (FMU). Perform the procedures of either Section 6.2.1 or 6.2.2:

6.2.1 Using Appendix I, determine the fractional model error (FMU) for each analyte.

6.2.2 Provide statistically determined uncertainties FMU for each analyte which are equivalent to two standard deviations at the 95% confidence level. Such determinations, if employed, must be based on mathematical examinations of the pertinent sample spectra (not the reference spectra alone). Include in the report of the analysis (see Section 7.0) a complete description of the determination of the concentration uncertainties.

6.3 Estimate Overall Concentration Uncertainty (OCU). Using Appendix J, determine the overall concentration uncertainty (OCU) for each analyte. If the OCU is larger than the required accuracy for any analyte, repeat Sections 4 and 6.

7.0 REPORTING REQUIREMENTS

[Documentation pertaining to virtually all the procedures of Sections 4, 5, and 6 will be required. Software copies of reference spectra and sample spectra will be retained for some minimum time following the actual testing.]

8.0 REFERENCES

- A) Standard Practices for General Techniques of Infrared Quantitative Analysis (American Society for Testing and Materials, Designation E 168-88).
- B) The Coblenz Society Specifications for Evaluation of Research Quality Analytical Infrared Reference Spectra (Class II); Anal. Chemistry **47**, 945A (1975); **Appl. Spectroscopy 44A**, pp. 211-215, 1990.
- C) Standard Practices for General Techniques for Qualitative Infrared Analysis, American Society for Testing and Materials, Designation E 1252-88.
- D) "Traceability Protocol for Establishing True Concentrations of Gases Used for Calibration and Audits of Continuous Emissions Monitors (Protocol Number 1)," June 1978, Quality Assurance Handbook for Air Pollution Measurement Systems, Volume III, Stationary Source Specific Methods, EPA-600/4-77-027b, August 1977.

APPENDIX A

DEFINITIONS OF TERMS AND SYMBOLS

A.1 Definitions of Terms

absorption band - a contiguous wavenumber region of a spectrum (equivalently, a contiguous set of absorbance spectrum data points) in which the absorbance passes through a maximum or a series of maxima.

absorption pathlength - in a spectrophotometer, the distance, measured in the direction of propagation of the beam of radiant energy, between the surface of the specimen on which the radiant energy is incident and the surface of the specimen from which it is emergent.

analytical region - a contiguous wavenumber region (equivalently, a contiguous set of absorbance spectrum data points) used in the quantitative analysis for one or more analyte.

Note: The quantitative result for a single analyte may be based on data from more than one analytical region.

apodization - modification of the ILS function by multiplying the interferogram by a weighing function whose magnitude varies with retardation.

background spectrum - the single beam spectrum obtained with all system components without sample present.

baseline - any line drawn on an absorption spectrum to establish a reference point that represents a function of the radiant power incident on a sample at a given wavelength.

Beers's law - the direct proportionality of the absorbance of a compound in a homogeneous sample to its concentration.

calibration transfer standard (CTS) gas - a gas standard of a compound used to achieve and/or demonstrate suitable quantitative agreement between sample spectra and the reference spectra; see Section 4.5.1.

compound - a substance possessing a distinct, unique molecular structure.

concentration (c) - the quantity of a compound contained in a unit quantity of sample. The unit "ppm" (number, or mole, basis) is recommended.

concentration-pathlength product - the mathematical product of concentration of the species and absorption pathlength. For reference spectra, this is a known quantity; for sample spectra, it is the quantity directly determined from Beer's law. The units "centimeters-ppm" or "meters-ppm" are recommended.

derivative absorption spectrum - a plot of rate of change of absorbance or of any function of absorbance with respect to wavelength or any function of wavelength.

double beam spectrum - a transmission or absorbance spectrum derived by dividing the sample single beam spectrum by the background spectrum.

Note: The term "double-beam" is used elsewhere to denote a spectrum in which the sample and background interferograms are collected simultaneously along physically distinct absorption paths. Here, the term denotes a spectrum in which the sample and background interferograms are collected at different times along the same absorption path.

fast Fourier transform (FFT) - a method of speeding up the computation of a discrete FT by factoring the data into sparse matrices containing mostly zeros.

flyback - interferometer motion during which no data are recorded.

Fourier transform (FT) - the mathematical process for converting an amplitude-time spectrum to an amplitude-frequency spectrum, or vice versa.

Fourier transform infrared (FTIR) spectrometer - an analytical system that employs a source of mid-infrared radiation, an interferometer, an enclosed sample cell of known absorption pathlength, an infrared detector, optical elements that transfer infrared radiation between components, and a computer system. The time-domain detector response (interferogram) is processed by a Fourier transform to yield a representation of the detector response vs. infrared frequency.

Note: When FTIR spectrometers are interfaced with other instruments, a slash should be used to denote the interface; e.g., GC/FTIR; HPCL/FTIR, and the use of FTIR should be explicit; i.e., FTIR not IR.

frequency, ν - the number of cycles per unit time.

infrared - the portion of the electromagnetic spectrum containing wavelengths from approximately 0.78 to 800 microns.

interferogram, $I(\sigma)$ - record of the modulated component of the interference signal measured as a function of retardation by the detector.

interferometer - device that divides a beam of radiant energy into two or more paths, generate an optical path difference between the beams, and recombines them in order to produce repetitive interference maxima and minima as the optical retardation is varied.

linewidth - the full width at half maximum of an absorption band in units of wavenumbers (cm^{-1}).

mid-infrared - the region of the electromagnetic spectrum from approximately 400 to 5000 cm^{-1} .

pathlength - see "absorption pathlength."

reference spectra - absorption spectra of gases with known chemical compositions, recorded at a known absorption pathlength, which are used in the quantitative analysis of gas samples.

retardation, σ - optical path difference between two beams in an interferometer; also known as "optical path difference" or "optical retardation."

scan - digital representation of the detector output obtained during one complete motion of the interferometer's moving assembly or assemblies.

scaling - application of a multiplicative factor to the absorbance values in a spectrum.

single beam spectrum - Fourier-transformed interferogram, representing the detector response vs. wavenumber.

Note: The term "single-beam" is used elsewhere to denote any spectrum in which the sample and background interferograms are recorded on the same physical absorption path; such usage differentiates such spectra from those generated using interferograms recorded along two physically distinct absorption paths (see "double-beam spectrum" above). Here, the term applies (for example) to the two spectra used directly in the calculation of transmission and absorbance spectra of a sample.

standard reference material - a reference material, the composition or properties of which are certified by a recognized standardizing agency or group.

Note: The equivalent ISO term is "certified reference material."

transmittance, T - the ratio of radiant power transmitted by the sample to the radiant power incident on the sample. Estimated in FTIR spectroscopy by forming the ratio of the single-beam sample and background spectra.

wavenumber, $\bar{\nu}$ - the number of waves per unit length.

Note: The usual unit of wavenumber is the reciprocal centimeter, cm^{-1} . The wavenumber is the reciprocal of the wavelength, λ , when λ is expressed in centimeters.

zero-filling - the addition of zero-valued points to the end of a measured interferogram.

Note: Performing the FT of a zero-filled interferogram results in correctly interpolated points in the computed spectrum.

A.2 Definitions of Mathematical Symbols

A, absorbance - the logarithm to the base 10 of the reciprocal of the transmittance (T).

$$A = \log_{10} \left(\frac{1}{T} \right) = -\log_{10} T \quad (1)$$

AAI_{i,m} - band area of the ith analyte in the mth analytical region, at the concentration (CL_i) corresponding to the product of its required detection limit (DL_i) and analytical uncertainty limit (AU_i) .

AAV_{i,m} - average absorbance of the ith analyte in the mth analytical region, at the concentration (CL_i) corresponding to the product of its required detection limit (DL_i) and analytical uncertainty limit (AU_i) .

ASC, accepted standard concentration - the concentration value assigned to a chemical standard.

ASCPP, accepted standard concentration-pathlength product - for a chemical standard, the product of the ASC and the sample absorption pathlength. The units "centimeters-ppm" or "meters-ppm" are recommended.

AU_i, analytical uncertainty limit - the maximum permissible fractional uncertainty of analysis for the ith analyte concentration, expressed as a fraction of the analyte concentration determined in the analysis.

AVT_m - average estimated total absorbance in the mth analytical region.

CKWN_k - estimated concentration of the kth known interferant.

CMA_i - estimated maximum concentration of the ith analyte.

CPOT_j - estimated concentration of the jth potential interferant.

DL_i, required detection limit - for the ith analyte, the lowest concentration of the analyte for which its overall fractional uncertainty (OFU_i) is required to be less than the analytical uncertainty limit (AU_i).

FC_m - center wavenumber position of the mth analytical region.

FAU_i, fractional analytical uncertainty - calculated uncertainty in the measured concentration of the ith analyte because of

errors in the mathematical comparison of reference and sample spectra.

FCU_i, fractional calibration uncertainty - calculated uncertainty in the measured concentration of the i^{th} analyte because of errors in Beer's law modeling of the reference spectra concentrations.

FPL_n - lower wavenumber position of the CTS absorption band associated with the m^{th} analytical region.

FFU_n - upper wavenumber position of the CTS absorption band associated with the m^{th} analytical region.

FL_n - lower wavenumber position of the m^{th} analytical region.

FMU_i, fractional model uncertainty - calculated uncertainty in the measured concentration of the i^{th} analyte because of errors in the absorption model employed.

FN_L - lower wavenumber position of the CTS spectrum containing an absorption band at least as narrow as the analyte absorption bands.

FN_U - upper wavenumber position of the CTS spectrum containing an absorption band at least as narrow as the analyte absorption bands.

FRU_i, fractional reproducibility uncertainty - calculated uncertainty in the measured concentration of the i^{th} analyte because of errors in the reproducibility of spectra from the FTIR system.

FU_n - upper wavenumber position of the m^{th} analytical region.

IAI_{j,n} - band area of the j^{th} potential interferant in the m^{th} analytical region, at its expected concentration (CPOT_j).

IAV_{i,n} - average absorbance of the i^{th} analyte in the m^{th} analytical region, at its expected concentration (CPOT_j).

ISC_{i or k}, indicated standard concentration - the concentration from the computerized analytical program for a single-compound reference spectrum for the i^{th} analyte or k^{th} known interferant.

kPa - kilo-Pascal (see Pascal).

L_s' - estimated sample absorption pathlength.

L_r - reference absorption pathlength.

L_s - actual sample absorption pathlength.

MAU_i - mean of the MAU_{im} over the appropriate analytical regions.

MAU_{i,m}, **minimum analyte uncertainty** - the calculated minimum concentration for which the analytical uncertainty limit (AU_i) in the measurement of the ith analyte, based on spectral data in the mth analytical region, can be maintained.

MIU_j, - mean of the MIU_{j,m} over the appropriate analytical regions.

MIU_{j,m}, **minimum interferant uncertainty** - the calculated minimum concentration for which the analytical uncertainty limit CPOT_j/20 in the measurement of the jth interferant, based on spectral data in the mth analytical region, can be maintained.

MIL, **minimum instrumental linewidth** - the minimum linewidth from the FTIR system, in wavenumbers.

Note: The MIL of a system may be determined by observing an absorption band known (through higher resolution examinations) to be narrower than indicated by the system. The MIL is fundamentally limited by the retardation of the interferometer, but is also affected by other operational parameters (e.g., the choice of apodization).

N_i - number of analytes.

N_j - number of potential interferants.

N_k - number of known interferants.

N_{scan} - the number of scans averaged to obtain an interferogram.

OFU_i - the overall fractional uncertainty in an analyte concentration determined in the analysis (OFU_i = MAX{FRU_i, FCU_i, FAU_i, FMU_i}).

Pascal (Pa) - metric unit of static pressure, equal to one Newton per square meter; one atmosphere is equal to 101,325 Pa; 1/760 atmosphere (one Torr, or one millimeter Hg) is equal to 133.322 Pa.

P_{min} - minimum pressure of the sampling system during the sampling procedure.

P_s' - estimated sample pressure.

P_r - reference pressure.

P_s - actual sample pressure.

RMS_m - measured noise level of the FTIR system in the mth analytical region.

RMSD, **root mean square difference** - a measure of accuracy determined by the following equation:

$$\text{RMSD} = \sqrt{\left(\frac{1}{n}\right) \sum_{i=1}^n e_i^2} \quad (2)$$

where:

n = the number of observations for which the accuracy is determined.

e_i = the difference between a measured value of a property and its mean value over the n observations.

Note: The RMSD value "between a set of n contiguous absorbance values (A_i) and the mean of the values" (A_M) is defined as

$$\text{RMSD} = \sqrt{\left(\frac{1}{n}\right) \sum_{i=1}^n (A_i - A_M)^2} \quad (3)$$

RSA_i - the (calculated) final concentration of the i^{th} analyte.

RSI_k - the (calculated) final concentration of the k^{th} known interferant.

t_{scan} , **scan time** - time used to acquire a single scan, not including flyback.

t_s , **signal integration period** - the period of time over which an interferogram is averaged by addition and scaling of individual scans. In terms of the number of scans N_{scan} and scan time t_{scan} , $t_s = N_{\text{scan}} t_{\text{scan}}$.

t_{ref} - signal integration period used in recording reference spectra.

t_{ss} - signal integration period used in recording sample spectra.

T_{ref} - absolute temperature of gases used in recording reference spectra.

T_s - absolute temperature of sample gas as sample spectra are recorded.

TP, Throughput - manufacturer's estimate of the fraction of the total infrared power transmitted by the absorption cell and transfer optics from the interferometer to the detector.

V_{ss} - volume of the infrared absorption cell, including parts of attached tubing.

W_{ik} - weight used to average over analytical regions k for quantities related to the analyte i ; see Appendix D.

Note that some terms are missing, e.g., BAV_m , OCU , $RMSS_m$, SUB_s ,
 SIC_i , SAC_i , S_s

APPENDIX B

IDENTIFYING SPECTRAL INTERFERANTS

B.1 General

B.1.1 Assume a fixed absorption pathlength equal to the value L_s' .

B.1.2 Use band area calculations to compare the relative absorption strengths of the analytes and potential interferants. In the m^{th} analytical region (FL_m to FU_m), use either rectangular or trapezoidal approximations to determine the band areas described below (see Reference A, Sections A.3.1 through A.3.3); document any baseline corrections applied to the spectra.

B.1.3 Use the average total absorbance of the analytes and potential interferants in each analytical region to determine whether the analytical region is suitable for analyte concentration determinations.

Note: The average absorbance in an analytical region is the band area divided by the width of the analytical region in wavenumbers. The average total absorbance in an analytical region is the sum of the average absorbances of all analytes and potential interferants.

B.2 Calculations

B.2.1 Prepare spectral representations of each analyte at the concentration $CL_i = (DL_i)(AU_i)$, where DL_i is the required detection limit and AU_i is the maximum permissible analytical uncertainty. For the m^{th} analytical region, calculate the band area (AAI_{im}) and average absorbance (AAV_{im}) from these scaled analyte spectra.

B.2.2 Prepare spectral representations of each potential interferant at its expected concentration ($CPOT_j$). For the m^{th} analytical region, calculate the band area (IAI_{jm}) and average absorbance (IAV_{jm}) from these scaled potential interferant spectra.

B.2.3 Repeat the calculation for each analytical region, and record the band area results in matrix form as indicated in Figure B.1.

B.2.4 If the band area of any potential interferant in an analytical region is greater than the one-half the band area of any analyte (i.e., $IAI_{jm} > 0.5 AAI_{im}$ for any pair ij and any m), classify the potential interferant as known interferant. Label the known interferants $k = 1$ to K . Record the results in matrix form as indicated in Figure B.2.

B.2.5 Calculate the average total absorbance (AVT_m) for each analytical region and record the values in the last row of the

matrix described in Figure B.2. Any analytical region where $AVT_m > 2.0$ is unsuitable.

FIGURE B.1 Presentation of Potential Interferant Calculations

		Analytical Regions			
		1	.	.	M
		<hr/>			
		Analyte Labels			
1		AAI_{11}	.	.	AAI_{1M}
.	
I		AAI_{I1}	.	.	AAI_{IM}
		<hr/>			
Potential Interferant Labels					
1		IAI_{11}	.	.	IAI_{1M}
.	
J		IAI_{J1}	.	.	IAI_{JM}

FIGURE B.2 Presentation of Known Interferant Calculations

		Analytical Regions			
		1	.	.	M
		<hr/>			
Analyte Labels					
1		AAI_{11}	.	.	AAI_{1M}
.	
I		AAI_{I1}	.	.	AAI_{IM}
		<hr/>			
Known Interferant Labels					
1		IAI_{11}	.	.	IAI_{1M}
.	
K		IAI_{K1}	.	.	IAI_{KM}
		<hr/>			
Total Average Absorbance		AVT_1		AVT_M	

APPENDIX C

ESTIMATING NOISE LEVELS

C.1 General

C.1.1 The root-mean-square (RMS) noise level is the standard measure of noise in this Protocol. The RMS noise level of a contiguous segment of a spectrum is defined as the RMS difference (RMSD) between the absorbance values which form the segment and the mean value of that segment (see Appendix A).

C.1.2 The RMS noise value in double-beam absorbance spectra is assumed to be inversely proportional to: (a) the square root of the signal integration period of the sample single beam spectra from which it is formed, and (b) to the total infrared power transmitted through the interferometer and absorption cell.

C.1.3 Practically, the assumption of C.1.2 allow the RMS noise level of a complete system to be estimated from the following four quantities:

- (a) RMS_{MAN} - the noise level of the system (in absorbance units), without the absorption cell and transfer optics, under those conditions necessary to yield the specified minimum instrumental linewidth, e.g., Jacquinot stop size.
- (b) t_{MAN} - the manufacturer's signal integration time used to determine RMS_{MAN} .
- (c) t_{SS} - the signal integration time for the analyses.
- (d) TP - the manufacturer's estimate of the fraction of the total infrared power transmitted by the absorption cell and transfer optics from the interferometer to the detector.

C.2 Calculations

C.2.1 Obtain the values of RMS_{MAN} , t_{MAN} , and TP from the manufacturers of the equipment, or determine the noise level by direct measurements with the completely constructed system proposed in Section 4.

C.2.2 Calculate the noise value of the system (RMS_{EST}) as follows:

$$RMS_{EST} = RMS_{MAN} \cdot TP \sqrt{\frac{t_{SS}}{t_{MAN}}} \quad (4)$$

APPENDIX D

ESTIMATING MINIMUM CONCENTRATION MEASUREMENT UNCERTAINTIES (MAU and MIU)

D.1 General

Estimate the minimum concentration measurement uncertainties for the i^{th} analyte (MAU_i) and j^{th} interferant (MIU_j) based on the spectral data in the m^{th} analytical region by comparing the analyte band area in the analytical region (AAI_{im}) and estimating or measuring the noise level of the system (RMS_{EST} or RMS_{SM}).

Note: For a single analytical region, the MAU or MIU value is the concentration of the analyte or interferant for which the band area is equal to the product of the analytical region width (in wavenumbers) and the noise level of the system (in absorbance units). If data from more than one analytical region is used in the determination of an analyte concentration, the MAU or MIU is the mean of the separate MAU or MIU values calculated for each analytical region.

D.2 Calculations

D.2.1 For each analytical region, set $\text{RMS} = \text{RMS}_{\text{SM}}$ if measured (Appendix G), or set $\text{RMS} = \text{RMS}_{\text{EST}}$ if estimated (Appendix C).

D.2.2 For each analyte associated with the analytical region, calculate

$$\text{MAU}_{im} = (\text{RMS}) (\text{DL}_i) (\text{AU}_i) \frac{(\text{FU}_m - \text{FL}_m)}{\text{AAI}_{im}} \quad (5)$$

D.2.3 If only the m^{th} analytical region is used to calculate the concentration of the i^{th} analyte, set $\text{MAU}_i = \text{MAU}_{im}$.

D.2.4 If a number of analytical regions are used to calculate the concentration of the i^{th} analyte, set MAU_i equal to the weighted mean of the appropriate MAU_{im} values calculated above; the weight for each term in the mean is equal to the fraction of the total wavenumber range used for the calculation represented by each analytical region. Mathematically, if the set of analytical regions employed is $\{m'\}$, then the MAU for each analytical region is

$$MAU_i = \sum_{k \in (m')} W_{ik} MAU_{ik} \quad (6)$$

where the weight W_{ik} is defined for each term in the sum as

$$W_{ik} = (FM_k - FL_k) \left(\sum_{p \in (m')} [FM_p - FL_p] \right)^{-1} \quad (7)$$

D.2.5 Repeat Sections D.2.1 through D.2.4 to calculate the analogous values MIU_j for the interferants $j = 1$ to J . Replace the value $(AU_i)(DL_i)$ in the above equations with $CPOT_j/20$; replace the value AAI_{im} in the above equations with IAI_{jm} .

APPENDIX E

DETERMINING FRACTIONAL REPRODUCIBILITY UNCERTAINTIES (FRU)

E.1 General

To estimate the reproducibility of the spectroscopic results of the system, compare the CTS spectra recorded before and after preparing the reference spectra. Compare the difference between the spectra to their average band area. Perform the calculation for each analytical region on the portions of the CTS spectra associated with that analytical region.

E.2 Calculations

E.2.1 The CTS spectra {R1} consist of N spectra, denoted by S_{1i} , $i=1, N$. Similarly, the CTS spectra {R2} consist of N spectra, denoted by S_{2i} , $i=1, N$. Each S_{ki} is the spectrum of a single compound, where i denotes the compound and k denotes the set {Rk} of which S_{ki} is a member. Form the spectra S_3 according to $S_{3i} = S_{2i} - S_{1i}$ for each i . Form the spectra S_4 according to $S_{4i} = [S_{2i} + S_{1i}] / 2$ for each i .

E.2.2 Each analytical region m is associated with a portion of the CTS spectra S_{2i} and S_{1i} , for a particular i , with lower and upper wavenumber limits FFL_m and FFU_m , respectively.

E.2.3 For each m and the associated i , calculate the band area of S_{4i} in the wavenumber range FFU_m to FFL_m . Follow the guidelines of Section B.1.2 for this band area calculation. Denote the result by BAV_m .

E.2.4 For each m and the associated i , calculate the RMSD of S_{3i} between the absorbance values and their mean in the wavenumber range FFU_m to FFL_m . Denote the result by $SRMS_m$.

E.2.5 For each analytical region m , calculate the quantity

$$FM_m = SRMS_m (FFU_m - FFL_m) / BAV_m$$

E.2.6 If only the m^{th} analytical region is used to calculate the concentration of the i^{th} analyte, set $FRU_i = FM_m$.

E.2.7 If a number p_i of analytical regions are used to calculate the concentration of the i^{th} analyte, set FRU_i equal to the weighted mean of the appropriate FM_m values calculated above. Mathematically, if the set of analytical regions employed is $\{m'\}$, then

$$FRU_i = \sum_{k \in \{m'\}} W_{ik} FM_k \quad (8)$$

where the W_{ik} are calculated as described in Appendix D.

APPENDIX F

DETERMINING FRACTIONAL CALIBRATION UNCERTAINTIES (FCU)

F.1 General

F.1.1 The concentrations yielded by the computerized analytical program applied to each single-compound reference spectrum are defined as the indicated standard concentrations (ISC's). The ISC values for a single compound spectrum should ideally equal the accepted standard concentration (ASC) for one analyte or interferant, and should ideally be zero for all other compounds. Variations from these results are caused by errors in the ASC values, variations from the Beer's law (or modified Beer's law) model used to determine the concentrations, and noise in the spectra. When the first two effects dominate, the systematic nature of the errors is often apparent; take steps to correct them.

F.1.2 When the calibration error appears non-systematic, apply the following method to estimate the fractional calibration uncertainty (FCU) for each compound. The FCU is defined as the mean fractional error between the ASC and the ISC for all reference spectra with non-zero ASC for that compound. The FCU for each compound shall be less than the required fractional uncertainty specified in Section 4.1.

F.1.3 The computerized analytical programs shall also be required to yield acceptably low concentrations for compounds with ISC=0 when applied to the reference spectra. The limits chosen in this Protocol are that the ISC of each reference spectrum for each analyte or interferant shall not exceed that compound's minimum measurement uncertainty (MAU or MIU).

F.2 Calculations

F.2.1 Apply each analytical program to each reference spectrum. Prepare a similar table as that in Figure F.1 to present the ISC and ASC values for each analyte and interferant in each reference spectrum. Maintain the order of reference file names and compounds employed in preparing Figure F.1.

F.2.2 For all reference spectra in Figure F.1, verify that the absolute value of the ISC's are less than the compound's MAU (for analytes) or MIU (for interferants).

F.2.3 For each analyte reference spectrum, calculate the quantity $(ASC - ISC)/ASC$. For each analyte, calculate the mean of these values (the FCU_i for the i^{th} analyte) over all reference spectra. Prepare a similar table as that in Figure F.2 to present the FCU_i and analytical uncertainty limit (AU_i) for each analyte.

FIGURE F.1

Presentation of Accepted Standard Concentrations (ASC's)
and Indicated Standard Concentrations (ISC's)

Compound Name	Reference Spectrum File Name	ASC (ppm)	ISC (ppm)					
			Analytes			Interferants		
			i=1.....I			j=1.....J		

FIGURE F.2

Presentation of Fractional Calibration Uncertainties (FCU's)
and Analytical Uncertainties (AU's)

Analyte Name	FCU (%)	AU (%)

APPENDIX G

MEASURING NOISE LEVELS

G.1 General

The root-mean-square (RMS) noise level is the standard measure of noise. The RMS noise level of a contiguous segment of a spectrum is the RMSD between the absorbance values that form the segment and the mean value of the segment (see Appendix A).

G.2 Calculations

G.2.1 Evacuate the absorption cell or fill it with UPC grade nitrogen at approximately one atmosphere total pressure.

G.2.2 Record two single beam spectra of signal integration period t_{ss} .

G.2.3 Form the double beam absorption spectrum from these two single beam spectra, and calculate the noise level RMS_{sm} in the M analytical regions.

APPENDIX H

DETERMINING SAMPLE ABSORPTION PATHLENGTH (L_s) AND FRACTIONAL ANALYTICAL UNCERTAINTY (FAU)

H.1 General

Reference spectra recorded at absorption pathlength (L_R), gas pressure (P_R), and gas absolute temperature (T_R) may be used to determine analyte concentrations in samples whose spectra are recorded at conditions different from that of the reference spectra, i.e., at absorption pathlength (L_s), absolute temperature (T_s), and pressure (P_s). Appendix H describes the calculations for estimating the fractional uncertainty (FAU) of this practice. It also describes the calculations for determining the sample absorption pathlength from comparison of CTS spectra, and for preparing spectra for further instrumental and procedural checks.

H.1.1 Before sampling, determine the sample absorption pathlength using least squares analysis. Determine the ratio L_s/L_R by comparing the spectral sets {R1} and {R3}, which are recorded using the same CTS at L_s and L_R , and T_s and T_R , but both at P_R .

H.1.2 Determine the fractional analysis uncertainty (FAU) for each analyte by comparing a scaled CTS spectral set, recorded at L_s , T_s , and P_s , to the CTS reference spectra of the same gas, recorded at L_R , T_R , and P_R . Perform the quantitative comparison after recording the sample spectra, based on band areas of the spectra in the CTS absorbance band associated with each analyte.

H.2 Calculations

H.2.1 Absorption Pathlength Determination. Perform and document separate linear baseline corrections to each analytical region in the spectral sets {R1} and {R3}. Form a one-dimensional array A_R containing the absorbance values from all segments of {R1} that are associated with the analytical regions; the members of the array are A_{Ri} , $i = 1, n$. Form a similar one-dimensional array A_s from the absorbance values in the spectral set {R3}; the members of the array are A_{si} , $i = 1, n$. Based on the model $A_s = rA_R + B$, determine the least-squares estimate of r , the value of r which minimizes the square error B^2 . Calculate the sample absorption pathlength $L_s = r'(T_s/T_R)L_R$.

H.2.2 Fractional Analysis Uncertainty. Perform and document separate linear baseline corrections to each analytical region in the spectral sets {R1} and {R4}. Form the arrays A_s and A_R as described in Section H.2.1, using values from {R1} to form A_R , and values from {R4} to form A_s . Calculate the values

$$\text{NRMS}_E = \sqrt{\sum_{i=1}^n \left[A_{Si} - \left(\frac{T_R}{T_S} \right) \left(\frac{L_S}{L_R} \right) \left(\frac{P_S}{P_R} \right) A_{Ri} \right]^2} \quad (9)$$

and

$$\text{IA}_{AV} = \frac{1}{2} \sum_{i=1}^n \left| A_{Si} + \left(\frac{T_R}{T_S} \right) \left(\frac{L_S}{L_R} \right) \left(\frac{P_S}{P_R} \right) A_{Ri} \right| \quad (10)$$

The fractional analytical uncertainty is defined as

$$\text{FAU} = \frac{\text{NRMS}_E}{\text{IA}_{AV}} \quad (11)$$

APPENDIX I

DETERMINING FRACTIONAL MODEL UNCERTAINTIES (FMU)

I.1 General

To prepare analytical programs for FTIR analyses, the sample constituents must first be assumed; the calculations in this appendix, based upon a simulation of the sample spectrum, verify the appropriateness of these assumptions. The simulated spectra consist of the sum of single compound reference spectra scaled to represent their contributions to the sample absorbance spectrum; scaling factors are based on the indicated standard concentrations (ISC) and measured (sample) analyte and interferant concentrations, the sample and reference absorption pathlengths, and the sample and reference gas pressures. No band-shape correction for differences in the temperature of the sample and reference spectra gases is made; such errors are included in the FMU estimate. The actual and simulated sample spectra are quantitatively compared to determine the fractional model uncertainty; this comparison uses the reference spectra band areas and residuals in the difference spectrum formed from the actual and simulated sample spectra.

I.2 Calculations

I.2.1 For each analyte (with scaled concentration RSA_i), select a reference spectrum SA_i with indicated standard concentration ISC_i . Calculate the scaling factors

$$RA_i = \frac{T_R L_S P_S RSA_i}{T_S L_R P_R ISC_i} \quad (12)$$

and form the spectra SAC_i by scaling each SA_i by the factor RA_i .

I.2.2 For each interferant, select a reference spectrum SI_k with indicated standard concentration ISC_k . Calculate the scaling factors

$$RI_k = \frac{T_R L_S P_S RSI_k}{T_S L_R P_R ISC_k} \quad (13)$$

and form the spectra SIC_k by scaling each SI_k by the factor RI_k .

I.2.3 For each analytical region, determine by visual inspection which of the spectra SAC_i and SIC_k exhibit absorbance bands within the analytical region. Subtract each spectrum SAC_i and SIC_k exhibiting absorbance from the sample spectrum S_s to form the spectrum SUB_s . To save analysis time and to avoid the introduction of unwanted noise into the subtracted spectrum, it is recommended that the calculation be made (1) only for those

spectral data points within the analytical regions, and (2) for each analytical region separately using the original spectrum S_s .

I.2.4 For each analytical region m , calculate the RMSD of SUB_s between the absorbance values and their mean in the region FFU_m to FFL_m . Denote the result by $RMSS_m$.

I.2.5 For each analyte i , calculate the quantity

$$FM_m = \frac{RMSS_m (FFU_m - FFL_m) AU_i DL_i}{AAI_i RSA_i} \quad (14)$$

for each analytical region associated with the analyte.

I.2.6 If only the m^{th} analytical region is used to calculate the concentration of the i^{th} analyte, set $FMU_i = FM_m$.

I.2.7 If a number of analytical regions are used to calculate the concentration of the i^{th} analyte, set FM_i equal to the weighted mean of the appropriate FM_m values calculated above. Mathematically, if the set of analytical regions employed is $\{m'\}$, then

$$FMU_i = \sum_{k \in \{m'\}} W_{ik} FM_k \quad (15)$$

where W_{ik} is calculated as described in Appendix D.

APPENDIX J

DETERMINING OVERALL CONCENTRATION UNCERTAINTIES (OCU)

The calculations in previous sections and appendices estimate the measurement uncertainties for various FTIR measurements. The lowest possible overall concentration uncertainty (OCU) for an analyte is its MAU value, which is an estimate of the absolute concentration uncertainty when spectral noise dominates the measurement error. However, if the product of the largest fractional concentration uncertainty (FRU, FCU, FAU, or FMU) and the measured concentration of an analyte exceeds the MAU for the analyte, then the OCU is this product. In mathematical terms, set $OFU_i = \text{MAX}\{\text{FRU}_i, \text{FCU}_i, \text{FAU}_i, \text{FMU}_i\}$ and $OCU_i = \text{MAX}\{\text{RSA}_i * OFU_i, \text{MAU}_i\}$.

APPENDIX K

SPECTRAL DE-RESOLUTION PROCEDURES

K.1 General.

High resolution reference spectra can be converted into lower resolution standard spectra for use in quantitative analysis of sample spectra. This is accomplished by truncating the number of data points in the original reference sample and background interferograms.

De-resolved spectra must meet the following requirements to be used in quantitative analysis.

(a) The resolution must match the instrument sampling resolution. This is verified by comparing a de-resolved CTS spectrum to a CTS spectrum measured on the sampling instrument.

(b) The Fourier transformation of truncated interferograms (and their conversion to absorbance spectra) is performed using the same apodization function (and other mathematical corrections) used in converting the sample interferograms into absorbance spectra.

K.2 Procedures

This section details three alternative procedures using two different commercially available software packages. A similar procedures using another software packages is acceptable if it is based on truncation of the original reference interferograms and the results are verified by Section K.3.

K.2.1 KVB/Analect Software Procedure - The following example converts a 0.25 cm^{-1} 100 ppm ethylene spectrum (cts0305a) to 1 cm^{-1} resolution. The 0.25 cm^{-1} CTS spectrum was collected during the EPA reference spectrum program on March 5, 1992. The original data (in this example) are in KVB/Analect FX-70 format.

(i) **decomp cts0305a.aif,0305dres,1,16384,1**

"decomp" converts cts0305a to an ASCII file with name 0305dres. The resulting ASCII interferogram file is truncated to 16384 data points. Convert background interferogram (bkg0305a.aif) to ASCII in the same way.

(ii) **compose 0305dres,0305dres.aif,1**

"Compose" transforms truncated interferograms back to spectral format.

(iii) **IG2SP 0305dres.aif,0305dres.ds,3,1,low cm^{-1} ,high cm^{-1}**

"IG2SP" converts interferogram to a single beam spectrum using Norton-Beer medium apodization, 3, and no zero filling, 1.

De-resolved interferograms should be transformed using the same apodization and zero filling that will be used to collect sample spectra. Choose the desired low and high frequencies, in cm^{-1} . Transform the background interferogram in the same way.

(iv) **DVDR 0305dres.dsrf,bkg0305a.dsrf,0305dres.dlf**

"DVDR" ratios the transformed sample spectrum against the background.

(v) **ABSB 0305dres.dlf,0305dres.dlf**

"ABSB" converts the spectrum to absorbance.

The resolution of the resulting spectrum should be verified by comparison to a CTS spectrum collected at the nominal resolution. Refer to Section K.3.

K.2.2 Alternate KVB/Analect Procedure -- In either DOS (FX-70) or Windows version (FX-80) use the "Extract" command directly on the interferogram.

(i) **EXTRACT CTS0305a.aif,0305dres.aif,1,16384**

"Extract" truncates the interferogram to data points from to 16384 (or number of data points for desired nominal resolution). Truncate background interferogram in the same way.

(ii) Complete steps (iii) to (v) in Section K.2.1.

K.2.3 Grams™ Software Procedure - Grams™ is a software package that displays and manipulates spectra from a variety of instrument manufacturers. This procedure assumes familiarity with basic functions of Grams™.

This procedure is specifically for using Grams to truncate and transform reference interferograms that have been imported into Grams from the KVB/Analect format. Table K-1 shows data files and parameter values that are used in the following procedure.

The choice of all parameters in the ICOMPUTE.AB call of step 3 below should be fixed to the shown values, with the exception of the "Apodization" parameter. This parameter should be set (for both background and sample single beam conversions) to the type of apodization function chosen for the de-resolved spectral library.

TABLE K-1. GRAMS DATA FILES AND DE-RESOLUTION PARAMETERS.

Desired Nominal Spectral Resolution (cm ⁻¹)	Data File Name	Parameter "N" Value
0.25	Z00250.sav	65537
0.50	Z00500.sav	32769
1.0	Z01000.sav	16385
2.0	Z02000.sav	8193

(i) **Import** using "File/Import" the desired *.aif file. Clear all open data slots.

(ii) **Open** the resulting *.spc interferogram as file #1.

(iii) **Xflip** - If the x-axis is increasing from left to right, and the ZPD burst appears near the left end of the trace, omit this step.

In the "Arithmetic/Calc" menu item input box, type the text below. Perform the calculation by clicking on "OK" (once only), and, when the calculation is complete, click the "Continue" button to proceed to step (iv). Note the comment in step (iii) regarding the trace orientation.

xflip:#s=#s(#0,#N)+50

(iv) **Run ICOMPUTE.AB** from "Arithmetic/Do Program" menu. Ignore the "subscripting error," if it occurs.

The following menu choices should be made before execution of the program (refer to Table K-1 for the correct choice of "N":)

First: **N** Last: **0** Type: **Single Beam**
Zero Fill: **None** Apodization: **(as desired)**
Phasing: **User**
Points: **1024** Interpolation: **Linear** Phase:
Calculate

(v) As in step (iii), in the "Arithmetic/Calc" menu item enter and then run the following commands (refer to Table 1 for appropriate "FILE," which may be in a directory other than "c:\mdgrams.")

setffp 7898.8805, 0 : loadspc "c:\mdgrams\ FILE" : #2=#s+#2

(vi) Use "Page Up" to activate file #2, and then use the "File/Save As" menu item with an appropriate file name to save the result.

K.3 Verification of New Resolution

K.3.1 Obtain interferograms of reference sample and background spectra. Truncate interferograms and convert to absorbance spectra of desired nominal resolution.

K.3.2 Document the apodization function, the level of zero filling, the number of data points, and the nominal resolution of the resulting de-resolved absorbance spectra. Use the identical apodization and level of zero filling when collecting sample spectra.

K.3.3 Perform the same de-resolution procedure on CTS interferograms that correspond with the reference spectra (reference CTS) to obtain de-resolved CTS standard spectra (CTS standards). Collect CTS spectra using the sampling resolution and the FTIR system to be used for the field measurements (test CTS). If practical, use the same pathlength, temperature, and standard concentration that were used for the reference CTS. Verify, by the following procedure that CTS linewidths and intensities are the same for the CTS standards and the test CTS.

K.3.4 After applying necessary temperature and pathlength corrections (document these corrections), subtract the CTS standard from the test CTS spectrum. Measure the RMSD in the resulting subtracted spectrum in the analytical region(s) of the CTS band(s). Use the following equation to compare this RMSD to the test CTS band area. The ratio in equation 7 must be no greater than 5 percent (0.05).

$$\frac{RMSS_i \times n(FFU_i - FFL_i)}{A_{CTS-test}} \leq .05 \quad (16)$$

RMSS=RMSD in the i^{th} analytical region in subtracted result, test CTS minus CTS standard.

n =number of data points per cm^{-1} . Exclude zero filled points.

FFU_i &= FFL_i =The upper and lower limits (cm^{-1}), respectively, of the analytical region.

$A_{test-CTS}$ =band area in the i^{th} analytical region of the test CTS.