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CENTER WING TANK RESIDUE TESTING
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by
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1.0 INTRODUCTION

At the request of Perkins Coei, Kreindler and Kreindler law firm, swab samples were collected from the scavenge pump inlet tube retrieved from the wreckage of TWA 800. These swab samples were collected at the Safety Board laboratory by a chemist from Artech Testing, L.L.C. All sampling supplies were supplied by Artech.

Duplicate wet and dry cotton swabs wipe samples were collected from pieces of the scavenge pump inlet tube. There were 2 sections of the inlet tube that were recovered during the accident investigation. These 2 sections were cut longitudinally by the Safety Board staff resulting in 2 pieces for each section. These 2 sections were labeled 65B and S3052. The S3052 section had a penetration hole in it. The pieces of inlet tube are shown in Figure 25 in Appendix 1. Methylene chloride solvent was used for the wet wipe samples. The Safety Board retained one set of samples (labeled with suffix -A) and the second set (with suffix -B) was retained by Artech[1]. In addition to the samples collected from the pieces of the inlet tube, Artech collected wipe samples from the center wing tank pieces CW236 and CW238 prior to metallurgical analysis. Wipe samples were taken from these two tank pieces after they were given to Artech. As a result, the Safety Board staff was unaware that wipe samples were taken from these CWT pieces until the this report was under preparation.

One set of the inlet tube wipe samples was analyzed by Artech and the second set was analyzed for the Safety Board by American University (AU). Artech chemical analyses were done independent of the Safety Board for the law firm cited above. American University provided the GC/MS data to the Safety Board staff for analysis. This report summarizes the results of testing from both laboratories.

The Artech report and fax supplements are attached to this report as Appendix 1 and 2. Detailed GC/MS data were not provided.

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[1] The samples labeled 65B also had a "-A" added to the numbering system for the Safety Board samples and a "-B" for the Artech samples.

2.0 AMERICAN UNIVERSITY SAMPLE PREPARATION

2.1 Preparation of American University

The samples that were retained by the Safety Board and the corresponding GC/MS report numbers from American University testing are provided in Table 1. Also included in this tabulation is the amount of solvent added to the samples by AU for analysis. The samples were prepared for GC-MS analysis by adding methylene chloride (Fisher Optima grade) to the sample vial. The dry swabs were extracted with 3 ml of methylene chloride. Since some of the cotton swabs had already been wetted prior to receipt, a smaller amount of methylene chloride (2 ml) was added to those. The vial was opened and the methylene chloride was added by means of a syringe. Once the cotton swab was wetted, a clean class stirring rod was used to lift the cotton swab off the bottom of the vial and squeeze the methylene chloride out of the cotton by pressing it against the wall of the vial. One microliter of the expressed methylene chloride was removed from the vial by syringe and injected into the GC-MS.

Table 1
Sample Identification and American University Sample Preparation

GC-MS Report Number	Identification Sample	Methylene Chloride added
Report 1	Wet Swab Sample 65B-A (Unbroken Piece of inlet tube)	2 ml
Report 3	Wet Swab Sample S3052-A	2 ml
Report 4	Dry Swab Sample Inlet Tube S3052-A (Piece with Hole)	3 ml
Report 5	Dry Blank – Nothing injected	Instrument blank
Report 6	Dry Swab Sample 65B Inlet Tube-A (Unbroken Piece)	3 ml
Report 7	Unlabeled Swab	2 ml
Report 8	Artech Methylene Chloride Blank	-----
Report 9	Dry Swab Sample Inlet Tube S3052-A	3 ml
Report 10	Cotton Swab Blank	3 ml
Report 11	Dry Swab 65 B-A	3ml

2.2 Analytical Procedures And Findings of American University

A Shimadzu 5100 GC-MS was used for the analysis. One micro-liter injections were made of each sample. A thirty meter DB-10 capillary column was used for the analysis. The MS (mass spectrometer) was tuned prior to analysis and a tuning profile is attached. The temperature program and other instrumental parameters are listed on an attached sheet labeled "GIRARDA.MET" (see Appendix 3). A GC trace and the corresponding mass spectra are attached as Appendix 4. Table 2 is a summary of the compounds identified from each analysis. Each report designated in Tables 1 and 2 correspond to chemical analysis (note that there is no report number 2). Table 2 shows a list of compounds that were identified for each of the GC peaks by comparing the mass spectra for this peak with the mass spectral library. This comparison is done via computer program.

Table 2
Compounds Identified In The Samples by American University

Report Number	Sample ID	Compounds Identified	Compound Class
1	Wet Swab 65B-A	Heneicosane, $C_{21}H_{44}$	Aliphatic hydrocarbon
		Tetratetacotane, $C_{44}H_{90}$	Aliphatic hydrocarbon
		Dodecanoic acid, 2-butoxy ester, $C_{18}H_{36}O_3$	Fatty acid ester
		2,4-bis (1-phenylethyl)phenol, $C_{22}H_{22}O$	Aromatic compound
3	Wet Swab Sample S3052-A	Tetratetacotane, $C_{44}H_{90}$	Aliphatic hydrocarbon
		4,4'-butylidenebis[2-(1,1dimethylethyl)-m-methyl-cresol, $C_{26}H_{38}O_2$	Aromatic hydrocarbon
		2,6,10-trimethyldodecane, $C_{15}H_{32}$	Aliphatic hydrocarbon
4	Dry Swab Sample Inlet Tube S3052-A (Piece with Hole)	Diethyl Phthalate, $C_{12}H_{14}O_4$	Phthalates are used as plasticizers (make plastics plyable)
		n-Decanoic Acid, $C_{10}H_{20}O_2$	Fatty acid
5	Dry Blank – Nothing injected	Caffeine, $C_8H_{10}N_4O_2$ –	Contaminant in instrument from prior analysis

Table 2, continued

Report Number	Sample ID	Compounds Identified	Compound Class
6	Dry Swab Sample 65 B Inlet Tube-A (Unbroken Piece)	Hydroxyacetaldehyde, $C_2H_4O_2$	Aldehyde
		n-Hexanedecanoic acid, $C_{16}H_{32}O_2$	Fatty acid
		9-octadecenamide, $C_{18}H_{35}NO$	Amide
		Dodecanoic acid, 2-butoxy ester, $C_{18}H_{36}O_3$	Aliphatic ester
7	Unlabeled Swab	n-Hexanedecanoic acid, $C_{16}H_{32}O_2$	Aliphatic acid
		Dodecanoic acid, 2-butoxy ester, $C_{18}H_{36}O_3$	Aliphatic ester
8	Artech Methylene Chloride Blank	Diethyl Phthalate, $C_{12}H_{14}O_4$	Solvent used by Artech to wipe residues
9	Dry Swab Sample Inlet Tube S3052-A	Diethyl Phthalate, $C_{12}H_{14}O_4$	Plasticizer
		N-(2-hydroxyphenyl)-Acetamide, $C_8H_9NO_2$	Amide
		n-Hexanedecanoic acid, $C_{16}H_{32}O_2$	Aliphatic acid
		4,7- dimethylundecene, $C_{13}H_{28}$	Aliphatic hydrocarbon
10	Cotton Swab Blank	Diethyl Phthalate, $C_{12}H_{14}O_4$	
		Tributyl phosphate, $C_{12}H_{27}O_4P$	
		n-Hexanedecanoic acid, $C_{16}H_{32}O_2$	Aliphatic acid
		Dodecanoic acid, 2-butoxy ester, $C_{18}H_{36}O_3$	Aliphatic ester
11	Dry Swab 65 B-A	Diethyl Phthalate, $C_{12}H_{14}O_4$	
		Tributyl phosphate, $C_{12}H_{27}O_4P$	
		n-Hexanedecanoic acid, $C_{16}H_{32}O_2$	Aliphatic acid
		Octanedecanoic acid, $C_{18}H_{36}O_2$	Aliphatic acid
		Nonadecanamide, $C_{19}H_{39}NO$	Amide
		2,7,10-trimethyldodecane, $C_{15}H_{32}$	Aliphatic hydrocarbon
		9-Octadeceneamide, $C_{18}H_{35}NO$	Amide
		2-Benzenedicarboxylic acid, diisoctyl ester, $C_{24}H_{38}O_4$	Large MW ester with aromatic character
		Dodecanoic acid, 2-butoxyethyl ester, $C_{18}H_{36}O_3$	Large MW aliphatic ester

2.3 DISCUSSION OF AMERICAN UNIVERSITY RESULTS

Three blanks or controls were run. They were; (1) a blank with nothing injected into the instrument (Report 5), (2) a sample of the methylene chloride used by Artech (Report 8), and (3) a cotton swab used by Artech to collect the residues (Report 10). The cotton swab was extracted with Fisher Optima grade methylene chloride. These blanks show the presence of a variety of compounds that cannot be attributed to residues that were on the surface of inlet tube parts at the time of the sampling but were contaminates that were present in the materials used for sample collection or were in the instrument itself. The instrument blank injection (Report 5) showed the presence of caffeine that is due to instrument contamination attributed to prior analysis. The methylene chloride control (Report 8) used by Artech to collect the wet swabs showed the presence of diethyl phthalate. Report 10 is a blank on the cotton used by Artech for collecting the residues. The cotton swab blank showed the presence of diethyl phthalate, tributyl phosphate, n-hexanedecanoic acid, and dodecanoic acid, 2-butoxy ester. Thus, all of these compounds are contaminants not related to the residue swabbed from the aircraft pieces. Diethyl phthalate is ubiquitous in the environment and can be expected. The source of the other compounds on the cotton swab shown in Report 10 is probably due to the processing of the cotton and/or could be due to handling without wearing gloves. Table 2 could be simplified by removing these compounds from the list of compounds identified in the samples collected from the aircraft.

Wet swab sample 65B-A that was collected from the unbroken inlet tube (Table 2, Report 1) contained 2 saturated long chain hydrocarbons (aliphatic compounds) and a phenolic hydrocarbon (aromatic compounds). The mass spectrum of these two peaks corresponding to the 2 long chain hydrocarbons matched reference spectra within 92%. A likely source of these 2 aliphatic compounds is the jet fuel. The mass spectra of the third unknown peak (phenol) when compared with the library mass spectra of compounds gave a match of 84%. This is not a high degree of match and suggests that the compound is not uniquely identified, but could be a similar compound. This compound has a high degree of aromatic character. This type of compound is used as a monomer in copolymer plastics such as Lexan™.

The dry swab sample from the unbroken inlet tube piece 65B-A (Report 6) showed the presence of an aliphatic acetaldehyde, an aliphatic long chain saturated acid, and a large molecular weight amide. The aldehyde is a low molecular weight species and is not likely to have been present immediately after the accident since it would have either been washed off in the ocean or vaporized off because of its low molecular weight. Therefore, it is most likely due to a post accident source. The amide is not likely to be present in the fuel and its source is unknown, but most likely a post accident contamination.

A second dry swab was analyzed (Report 11) that contained more compounds. This sample contained two long chain saturated aliphatic acids (C_{16} and C_{18}), two large molecular weight esters (C_{18} ,and C_{24} with a benzene ring), a saturated aliphatic hydrocarbon (C_{15}), and two large molecular weight aliphatic amides (C_{18} and C_{19}). A likely source of the aliphatic hydrocarbon is jet fuel. The large molecular weight acids are fatty acids and the most likely source of these are contamination from human hands. The source of the large molecular weight ester could also be related to the human contamination. The esters are formed from a reaction between the fatty acid and an alcohol. This reaction usually requires some external stimulus such as energy (heat) of some other chemical.

The compounds identified in the wet (Report 3) and dry (Report 9) sample S3052-A from the inlet tube consist of long chain aliphatic hydrocarbons, an aromatic hydrocarbon (cresol), and an amide. The presence of the aliphatic hydrocarbons is consistent with jet fuel as the source. The cresol could have originated from the fuel or could be a contamination from some plastic material. The source of the amide is unknown but not likely to be a fuel contaminant. It could be a decomposition product of the caffeine that was present in the instrument.

3.0 SUMMARY OF ARTECH RESULTS

Artech found some of the same chemicals as reported by American University. The Artech final report is attached as Appendix 1. This report generalized the results and conclusion without providing any analytical data or experimental conditions. This generalization, while not very informative, included statements such as; "long-chain branched hydrocarbons and Poly-Aromatic Hydrocarbons (PAHs)" were found. Consequently, more detailed chemical results were requested and this faxed report is attached as Appendix 2. The predominate residues found on the inlet tube pieces consisted of the aliphatic hydrocarbons. As stated earlier, Artech swabbed pieces CW236 and CW238. American University did not have swab samples taken from these pieces since these samples were collected at Artech and the Safety Board did not observe or participate in the collection process. Artech reported finding two large molecular weight aliphatic hydrocarbons in the wipe sample collected from C236; similar to those reported on the inlet tube pieces. However, they also reported the presence of perylene and a trichlorinated benzene compound on the C238 piece. Perylene is a PAH type of compound.

4.0 ANALYSIS OF ARTECH AND AMERICAN UNIVERSITY RESULTS

Table 3 compares the chemistry on pieces that were analyzed by both American University and Artech. As can be seen from this comparison, the aliphatic hydrocarbons and the aromatic compounds show some differences. However, the compounds have the same basic chemistry.

Table 3
Comparison of American University and Artech Results

Laboratory	Sample ID	Compounds Identified		
Artech	S3052-B	Eicosane ($C_{20}H_{42}$)or Heneicosane(($C_{21}H_{44}$)	Tricosane ($C_{23}H_{48}$)	Phenol, 4.4'-butylidene bis[2-(1,1-dimethyl-5] ($C_{26}H_{38}O_2$)
American U.	S3052-A	2,6,10-trimethyldodecane ($C_{15}H_{32}$)	Tetratetacotane ($C_{44}H_{90}$)	4.4'-butylidenebis[2-(1,1 dimethylethyl)-m-methyl-cresol ($C_{26}H_{38}O_2$)
Artech	65B-B	Eicosane	Heneicosane	Phenol ($C_{26}H_{38}O_2$) (see above)
American U.	65B-A	Heneicosane ($C_{21}H_{44}$)	Tetratetacotane ($C_{44}H_{90}$)	2.4-bis (1-phenylethyl)phenol, ($C_{22}H_{22}O$)

The two laboratories reported similar chemistry, but included some differences. Both laboratories report large molecular weight aliphatic hydrocarbons, which are the major components in Jet A fuel. Also, both report the presence of aromatic compounds. In this respect the laboratories are in agreement. However, there are some important differences as well. One example of this is that American University laboratory found the presence of fatty acids and some corresponding esters. Artech did not find the fatty acids or the esters. A closer review of the Artech data raises some questions about the quality of the mass spectra identification of GC peaks.

The tabulation of the peak number, retention time, and corresponding compounds with match percentage in the Artech report, Appendix 2, raises some questions about the compound identifications. For example, on sample S3052-B, two GC peaks eluting at 31.54 minutes and at 33.65 are identified as eicosane from the mass spectra. The degree of match with a mass spectra library is 95% and 92% respectively. A similar situation occurs on the swab sample taken from piece number C238-2. In this instance, two GC peaks were identified as perylene, one at 27.06 minutes and one at 27.23 minutes. These two sample were not analyzed by American University. It is very unlikely, if not impossible for a compound to elute at 2 different times in a single run with this type of analysis and this type of chemistry. This suggests at least two possible problems with these analyses; (1) the unknown GC compounds were very similar such that the software program that compares the mass spectra with a reference library is unable to uniquely identify the compounds, or (2) the mass spectra are insufficient (signal to noise is low because of very low concentrations of the unknown compounds) for a unique identification. The fact that the software program reports a relatively high degree of match is curious.

Compounds are eluted from the GC in a sequence that is dependent on the boiling point of the compound. The higher the boiling point the longer it takes for the compound to transverse the GC column. For example, eicosane, heneicosane, and tricosane have boiling points of 343, 356, and 380 C respectively. Thus these compounds will elute from the GC in this order. Eicosane would not elute at 2 different times. Nor would perylene or any other organic compound elute at two different times in the same gas chromatographic run. Perylene is particularly troublesome because, according to the reference literature, perylene does not boil under atmospheric condition but sublimes at 350 to 400 C. It has a **melting** point of about 275 C. For comparison purposes, eicosane has a melting point of 37 C. Although Artech did not report the chromatographic conditions, they reported in a phone conversation that the maximum chromatographic temperature was 300 C. Appendix 2 shows that the retention time (time it takes a compound to transit the GC column) of eicosane is 31.54 minutes and the retention time of perylene is about 27.06 minutes. Certainly, if perylene did go through the GC column it would not have a shorter retention time than eicosane since perylene has a melting point close to that of the boiling temperature of eicosane.

These issues raise serious doubts about the identification of peaks that has been identified as perylene and perhaps the halogenated hydrocarbon reported on the sample with perylene. The only way to confirm the presence of perylene would be to inject a perylene standard into the analytical system. This was not done so the results cannot be relied on with any scientific certainty. The American University analyses did confirm the presence of large molecular weight aliphatic hydrocarbons on samples S3052-A and on 65B-A. So in this respect, some of Artech findings have been confirmed by an independent analysis.

Artech classified the phenols (samples 65B-B and S3052-B) as being polyaromatic hydrocarbons (PAHs). Actually, PAHs are "polycyclic aromatic hydrocarbons". These compounds (PAHs) are generated during exposure of organic materials to a high temperature environment such as a fire. However, PAHs produced in high temperature environments consist of fused ring systems and not multi-ring aromatic compounds linked with carbon atoms that were reported as residues by American University and Artech on the pieces from the wreckage (samples S3052-A and -B and 65B A and B). Perylene would be classified as a PAH. However, Artech's identification of a GC peak as perylene is very doubtful given the properties of perylene and the analytical procedure used for the analysis. An example of a process that produces PAHs is smoking cigarettes and incineration. Many of the PAHs are considered to be carcinogenic although some have commercial applications such as dyes and pharmaceuticals.

In summary, the long chain aliphatic hydrocarbon identified on the cotton swabs that are the present as residues on the aircraft pieces can be associated with the fuel. The high molecular weight aliphatic acids (fatty acids) are most likely from finger grease as a result of handling of the pieces. The source of the aromatic compound identified by both laboratories on the aircraft pieces is not so clear. Jet fuel does contain some aromatic compounds, and the fuel is a possible source of these. However, these compounds should not be classified as PAHs. This aromatic compound is not likely to be the result of exposure of an aliphatic hydrocarbon (the predominate species in Jet fuel) to a high temperature environment. The source of the aromatic compounds could also be environmental contamination that occurred after the accident.