DOCKET NO. SA-516

EXHIBIT NO. 20H

NATIONAL TRANSPORTATION SAFETY BOARD WASHINGTON, D.C.

THE LABORATORY CHARACTERIZATION OF JET FUEL VAPOR UNDER SIMULATED FLIGHT CONDITIONS

 $(57$ pages)

THE LABORATORY CHARACTERIZATION OF **JET FUEL VAPOR UNDER SIMULATED FLIGHT CONDITIONS**

Prepared for the National Transportation Safety Board *(Order No.* **NTSB12-97-SP-0255)**

 $\overline{}$

Final Report

November. 1997

--

James E. Woodrow and James N. Seiber

Center for Environmental Sciences and Engineering University of **Nevada Reno, NV 89557-0187**

Abstract

The behavior of jet fuel and its vapor under different **sets** of conditions was studied as part of the National Transportation Safety Board's (NTSB's) investigation into the cause of the TWA Flight 800 accident (DCA96MA070; the crash of a 747- 13 1, N93 1 19). *An* important goal of this study was to provide technical information about the properties of jet fuel and its vapor under conditions that might have existed in the Flight *800* center wing fuel tank at the time of the explosion. Specifically, we wanted to address the question of fuel flammability under flight conditions at 14,000 feet. Headspace gas chromatography **was** used to measure component partial pressures and total vapor pressures for twelve jet fuel samples (Jet-A, Jet-Al) taken from the center **wing** tanks of commercial aircraft. Measurements were made at 32-33.5.40, and 50°C and at vapor volume-to-liquid volume *(VL)* ratios of 274, 136.5.26.5, and 1.2 for four of the samples. Measurements were also made at 40, 50, and 60° C and at V/L ratios of 274 (nearly empty tank; \sim 3 kg/m³) and 1.2 (half-filled tank; \sim 300-400 kg/m³) for eight of the samples. A pristine fuel sample obtained locally (Reno/Tahoe International Airport) from the sump of a refueling truck was subjected to all of these measurements **as** a comparison. The four fuel samples were taken from the center wing tank of flights arriving from Athens, Greece, soon after the Flight 800 incident in 1996. The additional eight samples were taken during Flight 800 simulation tests conducted by the NTSB during July, 1997. Our vapor pressure measurements indicated differential volatilization (i.e., weathering) of the samples taken from aircraft fuel tanks, resulting **in** the depletion of light ends (C5-Cs; decreasing mole percent) and the accumulation of the heavier ends $(C_9-C_{12};$ increasing mole percent), as reflected in the increased average molecular weights and lowered total vapor pressures of the samples. Despite these compositional changes, calculation of the effect of altitude on fuel vapor density for $V/L = 274$ (\sim 3 kg/m³) indicated that at about 14,000 feet, where the Flight 800 explosion took place, the center wing fuel tank would only have to be at ahout 50°C **(122F)** to create fueYair mass ratios (0.048-0.066) and fuel mole fractions (0.010**0.015) well within the flammability range, where the lower flammability limit would be at a fuel/& mass ratio** and **fuel mole fraction of about** 0.030 and **0.007, respectively.**

Acknowledgments

The authors gratefully acknowledge the technical assistance, helpful suggestions, and encouragement of Drs. Merritt Birky and Dan Bower, both with the National Transportation Safety Board, and professor Joseph Shepherd, California Institute of Technology, Graduate Aeronautical Laboratories. We also thank Dr. John Sagebiel, **Desert** Research Institute, for the many helpful discussions of his and our work related to the TWA 800 investigation. **This** report **was** submitted in fulfilment of Order #NTSB 12-97- SP-0255 by the Center for Environmental Sciences and Engineering, University of Nevada, Reno, under the sponsorship of the National Transportation Safety Board. Work was completed as of September 20,1997.

Table of Contents

List of Figures

page

V

List of Tables

Introduction

As part of the National Transportation Safety Boards (NTSB's) investigation into the cause of the TWA Flight 800 accident (DCA96MA070; crash of a 747-131, N93119), the behavior of jet fuel (Jet-A, Jet-Al) and its vapor under different **sets** of conditions was studied. A headspace gas chromatographic (HS-GC) method, described in detail in earlier reports (Woodrow and Seiber, 1988 and 1989), was used to determine component partial pressures and **total** vapor pressures of samples of jet fuel representative of the type of fuel used to fill the center wing tank in the TWA Flight 800 aircraft. Using this method, it was possible to accurately determine vapor pressures by modeling the jet fuel vapor, characterized by a complex mixture of hydrocarbons, with just a few n-alkane reference standards. **An** important goal of this study was to provide technical information about the properties of jet fuel and its vapor under conditions that might have existed in the Flight 800 center wing fuel tank at the time of the explosion. Specifically, we wanted to address the question of fuel flammability under flight conditions at 14,000 feet. It is hoped that this information will contribute to a better understanding of the nature of the accident.

Procedures

In May, 1997, the NTSB shipped to the University of Nevada (UNR) four liquid jet fuel samples, three of which were contained in glass bottles sealed with poly-seal screw caps and one contained in a metal can. These samples were taken during 1996 within a few months of the Flight 800 incident. During the test flights in July, 1997, eight additional liquid fuel samples were taken and shipped to UNR in sealed glass bottles. Sample designations and descriptions **are** summarized in Table 1. All samples were stored in a laboratory refrigerator at 1-2°C.

To generate the test flight samples 1-7, fuel was obtained from the outboard wing tank of a 747 aircraft that arrived from Athens, Greece, and 3,000 pounds was loaded into a fuel truck. Approximately 800 pounds was off-loaded from the truck to purge the fuel line on **the** truck, and 50 gallons was then pumped into the center wing tank of the test 747**Table 1. Liquid jet fuel samples supplied by the National Transportation Safety Board and Evergreen for vapor pressure determination and compositional analysis.**

100 series aircraft. This fuel remained on board for flights up through 001-03 (Table l), during which time different combinations of three environmental control system (ECS) packs were operated to cool the crew/passenger cabins. These **ECS** packs were located beneath the center wing fuel tank, and temperatures of the packs and of the fuel tank were monitored. For flight 001-04, the center wing tank was refueled with 6,000 pounds of **JFK** fuel and sample **8** was taken after completion of this flight. A brief description of the flight operations is summarized in Table 2. A much more detailed description of the entire flight test program is given by Bower (1997).

Into separate chilled 22 mL glass headspace vials (Perkin-Elmer, **Nonualk,** CT) were placed 0.08,0.16,0.80, and **10** mL of chilled liquid fuel samples, and the vials were immediately sealed with Teflon@-lined septa in crimped aluminum caps. These volumes of fuel represented vapor volume-to-liquid volume ratios of 274, 136.5,26.5, and 1.2, respectively (i.e., from an almost empty fuel tank to an approximately half-filled tank). The sealed samples were placed in an **HS-40** autosampler and injector (Perkin-Elmer), where they were thermostated at 30, 40, 50, and 60° C for 15-30 min. After the samples were thennostated, the **HS-40** automatically punctured the septa with a hollow sampling needle, the vials were pressurized to about 150 kPa, the equilibrated vapor was sampled for 0.01 min, the resulting vapor aliquot was injected onto a 60 m x 0.32 mm (id) DB-1 fused silica open tubular **(FSOT)** capillary column **(J&W** Scientific, Folsom, CA), and the chromatographed vapor was detected by a flame ionization detector. The column was held at 100° C for 4 min, after which time it was programmed at 2° /min to 140° C, where it was held for 1 min. The column carrier gas (helium) flow rate was about 3 mL/min , which means that for **an** injection time of 0.01 min, the volume of vapor sample injected was about 30 μ L (i.e., 3 mL/min x 0.01 min x 1000 μ L/mL).

The fuel samples were evaluated using a mixed hydrocarbon standard, which consisted of an equal volume mix of the normal alkanes pentane (C_5) through dodecane **(C₁₂).** Into separate chilled headspace vials were placed 1, 0.5, 0.25, and 0.1 μ L of the

					Liquid	Vapor
		Rotation	Highest	Landing	fuel	fuel
Date	Activity ^a	time	altitude, ft	time	samplingb	sampling ^C
7/14	Fuel added					
	to center					
	wing tank					
	(CWT)					
7/14	Flight	1237	17,500	1910	pre-flight	
					(11)	
7/15	Flight	1211	35,000	1628	pre- and	Taxi ^d
					post-flight	10,300 ft
					(H2, H3)	14,100 ft
7/15	TWA 800	2021	19,000	2257	pre- and	Taxie
	simulation				post-flight	10,100 ft
	flight				(H4, H5)	14,100 ft
7/16	Flight	1044	35,000	1628		
7/16	Flight	1955	17,500	2241	pre- and	Taxif
					post-flight	10,000 ft
					(H6, H7)	14,600 ft
7/17	CWT	1043	17,500	1452	post-flight	
	refueled				(#8)	

Table 2. Test flight operations (July, 1997) showing schedule for liquid and vapor fuel sampling. Times are EDT.

a *On* 7/14, the CWT **was** fueled with 50 gallons. On 7/17, the CWT was refueled with 6000 pounds of **JFK** fuel.

b **See** Table **1.**

 c Sagebiel (1997).

d Vapor sampling flight 1.

e Vapor sampling flight 2.

f Vapor sampling flight 3.

mixed standard and the sealed vials were processed in the same way as for the fuel samples. These volumes of mixed standard were low enough to allow the hydrocarbons to completely vaporize, so that eight separate vapor density standard curves could be generated for each spiking level. Using the gas chromatographic retention times of the hydrocarbon standards, the fuel vapor chromatograms were divided into eight subsections **(C5-C12),** each of which was approximately centered about the retention time of a hydrocarbon standard (Figure 1). The *peak* areas in each subsection were summed and treated **as** a single peak in the vapor density regression equations to calculate subsection vapor densities, which were used to calculate subsection partial pressures. All of the subsection partial pressures were summed to obtain **total** vapor pressures for the fuel samples.

Nine steel canister samples taken of fuel vapors during test flights on 7/15/97 and 7/16/97 (Table 2) were subsampled and analyzed using the same headspace method as for the liquid fuel samples. The canisters were sampled by allowing the pressure in the canisters (pressurized with zero air) to briefly flush the headspace vials with fuel vapor. The vials were immediately *sealed* and analyzed. Although the test flight samples were taken at temperatures in the range 42-51"C, the subsamples in sealed headspace vials were evaluated at an instrument temperature of 40°C. Eight liquid fuel samples, representing both pre- and post-flight conditions, were taken during the test flights and evaluated at 40, 50, and 60°C and at *VL* = 1.2 and 274 using the headspace method.

Some chemical characterization of the jet fuel vapor was performed using gas chromatography coupled with a mass-selective detector **(GC/MSD)** (Hewlett-Packard Company, San Fernando, CA). Using a gas-tight syringe, a $10 \mu L$ aliquot of fuel vapor equilibrated at 50°C was removed from a sealed headspace vial containing liquid fuel and injected into the **GClMSD** system. The injected sample was scanned over a mass range of 40-200, and fragmentation patterns of individual peaks were compared with the computer library entries to obtain the best matches.

Figure 1. Typical headspace gas chromatogram of Jet-A vapor showing standard retentions (carbon numbers 5-12) and subsections (vertical lines).

Results and Discussion

Analysis using headspace sampling and gas chromatography (GC) requires thermodynamic equilibrium between a condensed phase and its vapor phase in a sealed container so that **aliquots** of the vapor can be removed for quantitative GC analysis. For a liquid fuel mixture in equilibrium with its vapor in a sealed container, *GC* response of a component in the vapor is proportional to the vapor density. This means that measuring the *GC* response essentially measures the partial pressure if the instrument calibration factor is known. The calibration factor has a specific value for each component in the fuel mixture and depends on the characteristics of the detector used. However, the complex jet fuel mixture *can* be represented by a relatively small number of n-alkane reference standards and the properties of the standards can be attributed to the fuel mixture. In other words, a single n-alkane reference standard can be used to represent a summation of *GC* responses (subsection of the fuel GC) for a series of components in the jet fuel vapor. Then, the partial pressure corresponding to each subsection is obtained from the ideal gas law and the molecular weight of the n-alkane reference standard for each subsection. No correction for real gas behavior is necessary since total pressure in the sealed vials remains below about 304 kPa, above which gases become non-ideal.

The major objective of this study was to **use** the described method to determine component partial pressures and total vapor pressures of samples of jet fuel representative of the type of fuel used to fill the center wing **tank** in the **TWA** Flight 800 aircraft. The analytical instrumentation sampled the *sealed* vials using a pneumatic-balanced pressure principle which avoids the disadvantages associated with gas syringes, such **as** change of partial pressures of the volatiles due to reduced pressure in the syringe. In a typical operation, the septum of the thenostated sample was pierced by the hollow sampling needle, the vial was pressurized to 150 kPa, and then an aliquot of the headspace was injected onto the **FSOT** column using the vial pressure as the driving force.

The volumes of the mixed hydrocarbon standard were low enough to assure complete vaporization of the C_5-C_{12} hydrocarbons under the test conditions. For the higher molecular weight hydrocarbons (e.g., dodecane), especially at the lowest test temperature ($32-33.5^{\circ}$ C), $0.5 \mu L$ and less of the hydrocarbon mix was used to assure complete vaporization. The resulting vapor densities $\left(\frac{g}{m^3}\right)$ for the reference hydrocarbons were correlated with their gas chromatographic peak **areas** to generate eight individual calibration curves that were used to calculate subsection partial pressure. **These** eight regression equations were linear, with correlation coefficient (r^2) values close to unity. Each subsection summed *GC* peak area (5-12) was treated as an individual compound and was used in the appropriate subsection regression equation to calculate a vapor density. The molecular weights of the subsection reference hydrocarbons were then used to convert the mass densities to molar densities for **use** in the ideal gas equation.

Results for the four liquid fuel samples, removed from the center wing **tanks** of flights arriving from Athens, Greece, soon after the Flight *800* tragedy, are summarized in the **APPENDIX** as Tables A-1 through A-13, along with results for an unweathered fuel sample from the Reno/Tahoe International Airport. The results for the test flight vapor and the eight test flight liquid fuel samples **are** summarized in Tables A-14 through A-20, along with the results for the Reno fuel. Tables A-1 through A-13 and A-15 through A-20 include subsection and *total* vapor pressure (mbar), subsection mole percent, and subsection vapor density ($g/m³$) for the fuel vapor samples at 32-33.5°C, 40°C, 50, and 60°C and for four vapor volume-to-liquid volume (VL) ratios (i.e., 274, 136.5.26.5. 1.2). Based on the mole percent values, average molecular weights of the fuel vapor were computed for each VL ratio at each temperature. Table A-14 lists only the subsection mole percent and average molecular weight for the test flight vapor samples. Vapor pressures for these test flight vapor samples were not determined since subsampling of the steel canisters was done in a way only to transfer enough sample to measure by gas chromatography for relative comparisons. Because of the warm season (June-August), it

was not possible for our headspace instrument to equilibrate at 30[°]C. Furthermore, the fluctuating ambient temperature allowed us to evaluate only three of the five fuel samples at the lowest temperature. Finally, Table **3** is a partial listing of the compounds identified in jet fuel vapor, showing representatives of the chemical classes that make up jet fuel vapor. The classes included normal alkanes (pentane-dodecane), branched alkanes (2-methylbutane **through** 2,6-dimethyl-nonane), cyclic alkanes (methyl-cyclopentane through **1,2,4** trimethyl-cyclohexane), olefins (substituted pentene and octene), and aromatics (benzene derivatives).

The total saturation vapor pressures determined at **32,40,50,** and 60°C for the Reno fuel sample compared reasonably well with the published true vapor pressures (CRC, **1983),** estimated from a plot of vapor pressure **ys** temperature, and with pressure values determined by professor Joseph Shepherd at the California Institute of Technology (Shepherd et al., **1997)** (Table **4).** Correlation of the Reno fuel data in a Clausius-Clapeyron type equation gave the relationship

 $\ln P = 16.00968 - 4332/T$

where P is pressure (mbar) and T is **"K.** This compares with $\ln P = 15.56471 - 4191/T$

for the Shepherd et al. **(1997)** data.

In general for all of the liquid fuel samples at all test temperatures, relative vapor density (mole percent) for subsection carbon number *5* declined by a factor of **4-6** in going from an approximately half-filled tank ($V/L = 1.2$) to a nearly empty tank ($V/L = 274$), while the relative vapor density for subsection carbon number **9,** for example, remained essentially unchanged (up to **-26%** difference), **as** illustrated in Figure **2A** for Reno fuel. This behavior reflected a change from vapor saturation $(V/L = 1.2)$ to a situation of undersaturation $(V/L = 274)$, where the heavier vapor components predominated. This is also reflected in the higher average molecular weight for the undersaturation case compared to vapor saturation (Tables **A-8, A-13, A-19, A-20).** However, an increase in fuel

	Branched	Cyclic		
n-Alkanes	Alkanes	Alkanes	Olefins	Aromatics
pentane	2-me-butane	me-cyclopentane	2,3,4-trime-2-	
			pentene	toluene
hexane	2-me-pentane	$1,2$ -dime-		
		cyclopentane	2,6-dime-2-octene	p-xylene
octane	3-me-pentane	me-cyclohexane		m-xylene
nonane	3-me-hexane	$1,2$ -dime-		
		cyclohexane		o-xylene
decane	3-me-heptane	$1-et-3-me-$		
		cyclopentane		propyl benzene
undecane	4-me-octane			$1,2,3$ -trime-
		et-cyclohexane		benzene
dodecane	2-me-octane	$1,2,4$ -trime-		
		cyclohexane		
	2,6-dime-heptane			
	3-me-octane			
	3-et-2-me-heptane			
	3,6-dime-octane			
	2-me-nonane			
	2,6-dime-nonane			
	3-me-decane			

Table 3. Partial **list of compounds identified in the vapor of a jet fuel sample.**

Table **4.** Comparison of saturation vapor pressure values for Reno fuel with those for fuels evaluated **using** other methods.

a University of Nevada; fuel obtained from the Reno/Tahoe International Airport.

b California Institute of Technology; fuel obtained from LAX Airport (Shepherd et al., 1997).

c Values are for fuel formulated according to general guidelines (CRC, 1983).

Figure 2. Comparison of relative vapor density for Reno fuel at $V/L=1.2$ and 274 (A) and variation of relative vapor density with temperature for Reno fuel at V/L=274 (B).

temperature (33.5'C to **60°C)** decreased the relative vapor density for subsection carbon number 5 by only a factor of about 2 (1.8.2.4) and increased the relative vapor density for subsection carbon number 9 by only about 10% (8.7%, 10.4%) for both *VL* = 1.2 and 274. **This** is illustrated in Figure 2B for Reno fuel at **V/L** = 274. So, it appears that a change in liquid fuel volume by a factor of 125 has a greater effect on vapor composition than does a change in temperature of close to 30°C.

Compared to the test flight liquid fuel samples, the Reno sample had consistently higher **total** vapor pressures at the test temperatures and *VL* = 1.2 (i.e., saturation). This contrast was probably due to differential volatilization (weathering) of the other fuel samples, which were taken from actual aircraft fuel tanks. The effect of weathering was dramatically shown by both the liquid and vapor test flight samples, where subsection mole percent increased for the heavier vapor components **as** the fuels were allowed to vent at altitude (Tables A-14 through A-20). This effect for the liquid fuel samples is illustrated in Figure 3A for *test* flight samples 1-7 at 50°C (samples 4 and 5 are pre- and post-flight 800 simulation). Compared to the initial pre-flight sample 1, the other fuel samples showed substantially less relative vapor density for components $<\mathbb{C}_9$, but greater relative vapor density for components *S9.* Sample 7, which was taken at the end of a series of flights at altitude, showed the lowest relative vapor density for components $\langle C_9 \rangle$ and the greatest density for components *S9* compared to the other samples. Furthermore, partial pressures for sample 7 exceeded the pressures for sample **1** for components *S9,* indicating some compensation for losses of light ends due to increased mole fraction (partial pressure) of the heavier ends in the liquid fuel mixture (Figure 3B).

An example of the weathering effect on the vapor samples captured in steel canisters **is** shown in Figure 4A for the TWA 800 simulation flight (Table 2). Here we compare subsection mole percent for our test flight vapor sub-samples from the steel canisters (Table A-14) with the primary canister samples characterized by **DFU** (Sagebiel, 1997). Both sets of samples show reasonable agreement with regard to the effects of

Figure 3. Comparison of subsection mole percent for test flight samples at V/L=274 (A) and **comparison of subsection partial pressure for test flight samples at V/L=274 (B). (Table 2; Table A-18)**

Figure 4. Comparison of test flight vapor canister samples with the sub-sampled canisters (UNR) (A) and comparison of the test flight liquid samples (UNR) with the canister samples (B).

weathering and to subsection mole percent. These vapor samples reflected the behavior of the test flight liquid samples by showing subsection mole percent increases for the heavier vapor components **as** the fuels were allowed to vent at altitude. The shift in vapor composition to higher molecular weight components after each flight was reflected in an increased average molecular weight for each vapor sample (Table A-14). The overall average molecular weight of all nine of our canister sub-samples was 129.1, which compared well with the estimate by Sagebiel (1997) of 132.4. A comparison of the TWA 800 simulation flight liquid samples 4 and *5* (50°C. *VL* = 274; Table A-18) with the canister vapor samples taken during that flight and characterized by DRI is shown in Figure 4B. The vapor generated by the liquid samples 4 and *5* showed reasonable agreement with the **canister** samples in the weathering effect and subsection mole percent.

Despite compositional changes in the fuel due to weathering and handling, will the fuel still be flammable? To address this question, we used the vapor pressure, molecular weight, and mass density **data** for the liquid fuel samples (Tables A-4 through A-13 and A-15 through A-20) weathered in aircraft fuel tanks to calculate fuellair mass ratios and fuel mole fractions in air at *sea* level and at 14,000 feet for the nominal fuel loading *(VL* = 274; -3 kplm3). Tables *5* and 6 summarize the calculated results for these fuel samples at 40.50, and **60°C.** Inspection of the data indicates that, compared with a lower flammability limit of about 0.030 fuellair mass ratio or *0.007* mole fraction (Nestor, 1967), the fuels that were at least **at** 50°C not only exceeded these values but were well within the flammability range for the 14,000 foot altitude. The results in Table *5* (test flight liquid fuel samples) compare well with those of Sagebiel (1997), who computed comparable fuel/air mass ratios (0.048-0.054) and fuel mole fractions (0.010-0.012) for the 14,000 foot test flight fuel vapor samples that had temperatures in the range 42-47°C.

	Fuel/Air Mass Ratio ($V/L = 274$)					
		40° C		50° C		60° C
Sample	0 fta	14 kft b	0 fta	$14 \text{ kft}^{\text{b}}$	0 fta	14 kft ^b
	0.019	0.033	0.035	0.060	0.047	0.081
$\overline{2}$	0.015	0.026	0.030	0.052	0.041	0.071
$\overline{3}$	0.016	0.028	0.029	0.050	0.042	0.073
4	0.016	0.028	0.031	0.054	0.043	0.074
$\overline{5}$	0.016	0.028	0.028	0.048	0.041	0.071
$\overline{6}$	0.016	0.028	0.029	0.050	0.045	0.078
7	0.016	0.028	0.028	0.048	0.041	0.071
$\overline{\mathbf{8}}$	0.022	0.038	0.036	0.062	0.051	0.088
Reno	0.026	0.045	0.044	0.076	0.065	0.112
				Fuel Mole Fraction $(V/L = 274)$		
		40° C		50° C		60° C
Sample	0 ft c	14 kft ^d	0 ft c	14 kft^d	0 ft c	14 kftd
	0.004	0.007	0.008	0.014	0.010	0.017
$\overline{2}$	0.003	0.005	0.006	0.010	0.009	0.016
$\overline{3}$	0.003	0.005	0.006	0.010	0.009	0.016
$\overline{\bf 4}$	0.003	0.005	0.006	0.010	0.009	0.016
$\overline{\mathsf{5}}$	0.003	0.005	0.006	0.010	0.008	0.014
6	0.003	0.005	0.006	0.010	0.009	0.016
	0.003	0.005	0.006	0.010	0.008	0.014
$\overline{\mathbf{8}}$	0.005	0.009	0.008	0.014	0.011	0.019

Table *5.* FueVair **mass** ratios and fuel mole fractions for test flight samples at nominal loading.

a Atmospheric mass density (dry air): 1127.4 g/m^3 , 40°C; 1092.4 g/m^3 , 50°C; 1059.6 g/m^3 , 60°C.

b Mass ratios at 14 kft were determined by multiplying the ratios at sea level by 1 $atm/0.578$ atm.

^c Air molar density: 39.1 moles/m³, 40°C; 37.9 moles/m³, 50°C; 36.7 moles/m³, 60°C. Molar densities were determined from the average molecular weight of air (-28.84 g/mole) and the mass densities of air at the various temperatures.

d Fuel mole fractions at **14** kft were determined by multiplying the fractions at sea level by 1 atm/0.578 atm.

		Fuel/Air Mass Ratio ($V/L = 274$)		
		40° C		50°C
Sample	0 fta	14 kft ^b	0 fta	14 kft ^b
1296-683	0.025	0.043	0.038	0.066
1296-683	0.021	0.036	0.038	0.066
(center tank)				
1296-684	0.020	0.035	0.034	0.059
1296-684	0.018	0.031	0.034	0.059
(sump)				
Reno	0.026	0.045	0.044	0.076
			Fuel Mole Fraction ($V/L = 274$)	
		40° C		50° C
Sample	0 ft c	$14 \mathrm{kf}t$ ^d	0 ft c	14 kft
1296-683	0.006	0.010	0.009	0.015
1296-683	0.005	0.008	0.009	0.015
(center tank)				
1296-684	0.005	0.008	0.008	0.014
1296-684	0.004	0.007	0.008	0.014
(sump)				

Table 6. FueVair **mass** ratios and fuel mole fractions for Athens fuel at nominal loading.

a Atmospheric mass density (dry air): 1127.4 g/m3,40"C; 1092.4 **g/m3,** 50°C.

b Mass ratios at **14** kft were determined by multiplying the ratios at sea level by 1 atm/0.578 atm.

^c Air molar density: 39.1 moles/m³, 40° C; 37.9 moles/m³, 50° C. Molar densities were determined from the average molecular weight of air (-28.84 g/mole) and the mass densities of air at the various temperatures.

d Fuel mole fractions at 14 kft were determined by multiplying the fractions at sea level by 1 atm/0.578 atm.

Conclusions

1. The effect of weathering on jet fuels (Jet-A, Jet-Al) in the center wing tank (CWT) was reflected in a change in fuel composition, leading to lower total vapor pressures and higher average molecular weights. Total vapor pressure of the fuels declined and average molecular weight increased with weathering when the fuels were exposed to typical flight conditions in the CWT. The ability of the headspace gas chromatography **(HS-GC)** method to measure fuel component properties showed that these changes in fuel properties were due primarily to changes in fuel composition through the loss of the more volatile components $($C₉$)$ and enrichment in the less volatile, higher molecular weight components ($\geq C_9$).

2. Weathered jet fuel in the CWT still exceeded the lower flammability limit at 14,000 feet and -50°C. Although weathered fuel had lower total vapor pressures, partial pressures of the higher molecular weight components were greater than pressures for the **same** components in unweathered fuel under the same conditions. This helped to partly off-set the effects of **losses** of the more volatile components by generating enough vapor mass at -50°C and *-0.58* atmospheres **(14,000** feet) to maintain flammability, **as** was indicated by calculations of fuel/air mass ratio and fuel mole fraction in air.

3. Jet fuel in the CWT consisted primarily of alkanes, followed by substituted aromatics and then olefim. Of the alkanes (normal, branched, and cyclic), branched alkanes predominated. These classes of compounds and order of occurrence compare well with analyses reported by others (Sagebiel, 1997; **NTSB,** 1997). For example, the Athens fuel, used to fill the CWT of TWA **800,** has been reported to consist of over *80%* alkanes, with aromatics amounting to only about 17% by volume and olefins making up about *0.5%* by volume **(NTSB,** 1997). Although the jet fuels in this study underwent compositional changes through venting of the CWT at altitude, the weathered fuels were still characterized by these classes of compounds.

4. HS-GC *is* **a good and reliable method for modeling the behavior of jet fuels and their vapors under simulated flight conditions.** It was not necessary to know the precise composition of the jet fuels, but these complex mixtures could be approximated with n-alkane reference standards whose GC retention times spanned the chromatogram envelopes of the fuels. Of critical importance is the fact that the HS-GC method will respond only to hydrocarbons and will be unaffected by non-hydrocarbon constituents, such **as** dissolved air, water, etc. This method was validated by obtaining saturation vapor pressures at several temperatures for unweathered fuel (Reno) that were essentially the same **as** pressure values obtained for unweathered fuels using other, unrelated methods (Shepherd et al., 1997; CRC, 1983). Furthermore, the good comparison between our test flight liquid and vapor samples and the vapor samples characterized by Sagebiel(1997) and the good agreement between his and our fuel/air mass ratio and fuel mole fraction calculations lend further support to the HS-GC method as a reliable alternative to other methods.

References

Bower, D. **1997.** *Flight Test Group Chairman's Factual Report of Investigation.* National Transportation Safety Board, November.

CRC. **1983.** *Handbook of Aviation Fuel Properties.* Coordinating Research Council, **Atlanta,** Georgia. Report No. **530** (Figure 20, pg. 46).

Nestor, L. **1%7.** *Investigation of Turbine Fuel Flammability within Aircrafr Fuel Tanks.* Final Report DS-67-7, Naval Air Propulsion Test Center, Naval **Base,** Philadelphia.

NTSB. **1997.** Private communication.

Sagebiel, J.C. 1997. *Sampling and Analysis of Vapors from the Center Wing Tank of a Test Boeing 747-IOOAircrafr.* Final Report to the National Transporkition Safety Board, November.

Shepherd, J.E.; J.C. Krok; J.J. Lee. 1997. *Jet A Explosion Experiments: Laboratory Testing.* **Report prepared for the National Transportation Safety Board under Order NTSB 12-97-SP-0127, June 26.**

Woodrow, J.E., and J.N. Seiber. 1988. Vapor-pressure measurement of complex hydrocarbon mixtures by headspace gas chromatography. *Journal of Chromatography,* **455~53-65.**

Woodrow, J.E., and J.N. Seiber. 1989. *Evaluation of a Method for Determining Vapor Pressures of Petroleum Mixtures by Headrpace* **Gas** *Chromatography.* **Final Report to the California** *Air* **Resources Board (Contract #A6-178-32), September.**

APPENDIX

Table A-1. Headspace GC results for jet-a fuel sample 1296-683 at 33.5°C, except for V/L = 1.2 which was determined at 32°C (total pressures are averages [\pm SD] of three determinations).

l,

a V/L = vapor volume-to-liquid volume ratio. \overline{b} Determined at 32°C.

Table A-2. Headspace GC results for jet-a fuel sample 1296-684 at 33.5°C, except for V/L = 1.2 which was determined at 32°C (total pressures are averages [\pm SD] of three determinations).

 $\frac{a}{a}$ V/L = vapor volume-to-liquid volume ratio. $\frac{b}{b}$ Determined at 32°C.

 \overline{a} V/L = vapor volume-to-liquid volume ratio. \overline{b} Determined at 32°C.

Table A-4. Headspace GC results for jet-a fuel sample 1296-683 at 40°C (total pressures are averages [±SD] of three determinations).

a V/L = vapor volume-to-liquid volume ratio.

l,

Table A-5. Headspace GC results for jet-a fuel sample 1296-683 (center fuel tank) at 40°C (total pressures are averages [±SD] of three determinations).

 $\left(\overline{36}\right)$

Table A-6. Headspace GC results for jet-a fuel sample 1296-684 at 40°C (total pressures are averages [±SD] of three determinations).

 \overline{a} V/L = vapor volume-to-liquid volume ratio.

28

Table A-7. Headspace GC results for jet-a fuel sample 1296-684 (sump) at 40°C (total pressures are averages [±SD] of three determinations).

a V/L = vapor volume-to-liquid volume ratio.

29

Table A-8. Headspace GC results for Reno jet-a fuel sample (taken from sump of fuel truck) at 40°C (total pressures are averages [±SD] of three determinations).

 α V/L = vapor volume-to-liquid volume ratio.

 $30\,$

Table A-9. Headspace GC results for jet-a fuel sample 1296-683 at 50°C (total pressures are averages [±SD] of three determinations).

 $\sqrt{\frac{4}{\pi}}$

Table A-10. Headspace GC results for jet-a fuel sample 1296-683 (center fuel tank) at 50°C (total pressures are averages [±SD] of three determinations).

Table A-11. Headspace GC results for jet-a fuel sample 1296-684 at 50°C (total pressures are averages [±SD] of three determinations).

 γ

Table A-12. Headspace GC results for jet-a fuel sample 1296-684 (sump) at 50°C (total pressures are averages [±SD] of three determinations).

 $\ddot{}$

 $\sqrt{3}$

Table A-13. Headspace GC results for Reno jet-a fuel sample (taken from sump of fuel truck) at 50°C (total pressures are averages [±SD] of three determinations).

 \mathcal{L}_{12}

Table A-14. Subsection mole percent and average molecular weight for test flight vapor samples taken on 7/15/97 and 7/16/97.

 $\widetilde{\mathcal{G}}$

 $\frac{1}{2}$

36

 $\frac{1}{2}$, $\frac{1}{2}$

Table A-15. Headspace GC results for test flight samples at 40°C (10 mL [V/L = 1.2]).

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

Table A-15, cont.

^a Reno/Tahoe International Airport. Taken from sump of fuel truck.

 $\alpha_{\rm m}$

a Reno/Tahoe International Airport. Taken from sump of fuel truck. ^b No peaks detected.

a Reno/Tahoe International Airport. Taken from sump of fuel truck. ^b No peaks detected.

 \mathcal{L}

L

a Reno/Tahoe International Airport. Taken from sump of fuel truck. ^b No peaks detected.

^a Reno/Tahoe International Airport. Taken from sump of fuel truck.

41

^a Reno/Tahoe International Airport. Taken from sump of fuel truck.

 $\ddot{}$

 $- -$

Table A-18. Headspace GC results for test flight samples at 50°C (80 µL [V/L = 274]).

 $\hat{\boldsymbol{\beta}}$

a Reno/Tahoe International Airport. Taken from sump of fuel truck. ^b No peaks detected.

 \overline{C}

43

a Reno/Tahoe International Airport. Taken from sump of fuel truck. ^D No peaks detected.

 $\ddot{\cdot}$

Table A-19. Headspace GC results for test flight samples at 60°C (10 mL [V/L = 1.2]).

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

.

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

a Reno/Tahoe International Airport. Taken from sump of fuel truck.

Table A-20, cont.

a Reno/Tahoe International Airport. Taken from sump of fuel truck.