

**DOT/FAA/AR-02/96**

Office of Aviation Research  
Washington, D.C. 20591

# **Determination of Fuel/Air Mass Ratios for Jet Fuels at Their Flash Point Temperatures**

September 2006

Final Report

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1. Report No. <b>DOT/FAA/AR-02/96</b>		2. Government Accession No.		3. Recipient's Catalog No.	
4. Title and Subtitle <b>DETERMINATION OF FUEL/AIR MASS RATIOS FOR JET FUELS AT THEIR FLASH POINT TEMPERATURES</b>				5. Report Date <b>September 2006</b>	
				6. Performing Organization Code	
7. Author(s) <b>James E. Woodrow</b>				8. Performing Organization Report No.	
9. Performing Organization Name and Address <b>Center for Environmental Sciences and Engineering University of Nevada Reno, NV 89557-0187</b>				10. Work Unit No. (TRAIS)	
				11. Contract or Grant No.	
12. Sponsoring Agency Name and Address <b>U.S. Department of Transportation Federal Aviation Administration Office of Aviation Research and Development Washington, DC 20591</b>				13. Type of Report and Period Covered <b>Final Report</b>	
				14. Sponsoring Agency Code <b>ANM-100</b>	
15. Supplementary Notes <b>The Federal Aviation Administration Airport and Aircraft Safety R&amp;D Division Technical Monitor was Skip Byrnes.</b>					
16. Abstract <p>The goal of this project was to determine fuel vapor densities and, ultimately, fuel-to-air mass ratios (FAMRs) for 11 commercial jet fuels at their flash point temperatures. The vapor composition of each fuel sample was modeled at each flash point temperature, rounded to the nearest whole value, using an alkane reference standard (pentane), with the results expressed as total vapor density for each fuel sample. In addition, the liquid composition of each fuel sample was modeled using 16 alkane reference standards (C<sub>5</sub>-C<sub>20</sub>), again with the results expressed as total vapor density. From these vapor density values, FAMRs were derived. From the determination of vapor composition, the measured vapor densities fell in the range 44.0-54.0 g/m<sup>3</sup>, depending on the flash point temperature, and the FAMRs fell in the range 0.041-0.047, with an average value of 0.044 and a percent relative standard deviation (%RSD) of 4.5. Based on the liquid composition, vapor densities calculated for the exact flash point temperatures fell in the range 46.5-50.4 g/m<sup>3</sup>, and the FAMRs fell in the range 0.043-0.045, with an average value of 0.044 and a %RSD of 2.3. These results demonstrate that the FAMR is a constant value at the flash point and this value is 0.044.</p>					
17. Key Words <b>Jet fuel property, Vapor density, Ullage</b>			18. Distribution Statement <b>This document is available to the public through the National Technical Information Service (NTIS) Springfield, Virginia 22161.</b>		
19. Security Classif. (of this report) <b>Unclassified</b>		20. Security Classif. (of this page) <b>Unclassified</b>		21. No. of Pages <b>23</b>	22. Price

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## EXECUTIVE SUMMARY

The characteristics of 11 Jet A fuel samples, taken at commercial airports were determined as part of the an investigation into the properties of commercial jet fuels. For the fuel vapor, a headspace gas chromatographic (HS-GC) method was used to determine fuel vapor density at fuel flash point by injecting a fixed volume (~30  $\mu\text{L}$ ) of equilibrated fuel vapor into an analytical instrument and monitoring the hydrocarbons in the vapor using a flame ionization detector. Using the HS-GC method, it was possible to reliably determine vapor densities by modeling the jet fuel vapor, characterized by a complex mixture of 140+ hydrocarbons, with the use of a single alkane ( $\text{C}_5$ ) reference standard. This was done by dividing the fuel vapor chromatogram into eight subsections, each of which corresponded to the retention time of a pure alkane reference. For example, the first subsection corresponded to a 5-carbon reference, the next subsection to a 6-carbon reference, etc. (i.e.,  $\text{C}_5\text{-C}_{12}$ ). The peaks falling into each subsection were summed, and each summed area was treated as an individual peak in the  $\text{C}_5$  standard regression equation (vapor density vs GC peak area) to obtain fuel vapor density for each subsection. The subsection vapor densities were then summed to obtain total vapor density for the fuels at their flash point temperatures. The liquid composition of each fuel sample was also modeled, except that 16 alkane reference standards ( $\text{C}_5\text{-C}_{20}$ ) were used instead of a single standard, as in the case for the HS-GC method. Each fuel sample was injected, as the neat liquid, into an analytical instrument and each of the 400+ hydrocarbon components was monitored using a flame ionization detector. The fuel chromatograms were divided into 16 subsections, each corresponding to the retention time of a pure alkane reference, as in the case for the HS-GC method. Sixteen regression equations, one for each subsection ( $\text{C}_5\text{-C}_{20}$ ), were generated by correlating hydrocarbon mass injected with GC response, expressed as peak area. The peaks falling into each subsection were summed, and each summed area was treated as an individual peak in the corresponding regression equation to obtain subsection mass for the liquid fuels. Each subsection mass was converted to number of moles by dividing subsection mass by the molecular weight of the hydrocarbon reference corresponding to the subsection. From this, mole fraction was derived. Unlike the HS-GC method, which directly measured fuel vapor density, subsection mole fraction and subsection reference hydrocarbon saturation vapor pressure were used with Raoult's law to calculate subsection partial pressure, assuming ideal behavior (e.g., activity coefficient = unity). Vapor density was calculated from the latter value using the ideal gas law.

Air mass density ( $\text{g}/\text{m}^3$ ) was correlated with temperature, and air mass densities at the fuel flash point temperatures were derived. Using these calculated values plus the fuel vapor mass density values determined using the HS-GC and liquid assay methods, fuel-to-air mass ratios (FAMRs) were calculated at the fuel flash point temperatures. From the HS-GC method, the measured vapor densities fell in the range 44.0-54.0  $\text{g}/\text{m}^3$ , depending on the flash point temperature (rounded to the nearest whole value), and the FAMRs fell in the range 0.041-0.047, with an average value of 0.044 and a percent relative standard deviation (%RSD) of 4.5. From the liquid fuel method, vapor densities calculated for the exact flash point temperatures fell in the range 46.5-50.4  $\text{g}/\text{m}^3$ , and the FAMRs fell in the range 0.043-0.045, with an average value of 0.044 and a %RSD of 2.3.

These results demonstrate that, for the selected jet fuels, the FAMR was a constant value at the flash point and that this value was 0.044. Both the HS-GC and liquid fuel methods gave results that were essentially equivalent, but the liquid fuel results appeared to have better precision.

Using Raoult's law, the liquid fuel results can be used to calculate fuel vapor properties at any given temperature, if the saturation vapor pressures for the reference hydrocarbons at those temperatures are known; but, the HS-GC results were unique to the fuel sample test conditions. The fuel property results from both the HS-GC and liquid fuel methods can be used in a comparative way to explain the differences in fuel flash points.

## INTRODUCTION

The characteristics of selected Jet A fuel samples taken at commercial airports were determined as part of an investigation into the properties of commercial jet fuels. For the fuel vapor, a headspace gas chromatographic method, described in detail in earlier reports (Woodrow and Seiber, 1988, 1989, and 1997), was used to determine fuel vapor density and, ultimately, the fuel-to-air mass ratio (FAMR) for 11 commercial jet fuel samples. Using this method, it was possible to reliably determine vapor densities by modeling the jet fuel vapor, characterized by a complex mixture of hydrocarbons, with the use of a normal alkane reference standard. This modeling approach was also applied to the liquid fuels, as well to determine vapor densities, and FAMR, as a way to confirm the vapor results. An important goal of this study was to provide technical information about jet fuel properties that could be used to describe fuel behavior under typical flight conditions.

## PROCEDURES

In late January, 2000, the Federal Aviation Administration (FAA) William J. Hughes Technical Center, Atlantic City, NJ, shipped to the University of Nevada (UNR) 11 Jet A fuel samples selected to represent a range of flash point temperatures (FAA sample Nos: 204, 211, 225, 270, 298, 344, 362, 366, 367, 389, and 395). Immediately upon arrival at UNR, each sample was logged in and placed in a cold explosion-proof refrigerator (0-1°C) for storage. These samples were subjected to the following analytical methods to determine vapor density and the FAMR for the fuels at their respective flash point temperatures.

### HEADSPACE (VAPOR) METHOD.

Volumes of either 5 mL or 10 mL of chilled liquid fuel samples were placed into separate 22 mL glass headspace vials (Perkin-Elmer, Norwalk, CT) chilled in ice, the vials were immediately sealed with Teflon<sup>®</sup>-lined septa in crimped aluminum caps. The sealed samples were placed in an HS-40 autosampler and injector (Perkin-Elmer), where they were thermostated at the various fuel flash point temperatures for 30 min. After the samples were thermostated, the HS-40 automatically punctured the septa with a hollow sampling needle, the vials were pressurized to about 113-114 kPa, the equilibrated vapor was sampled for 0.04 min, the resulting vapor aliquot was injected onto a 60 m x 0.32 mm (i.d.) 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 160°C, where it was held for 1 min. The column carrier gas (helium) flow rate was about 2 mL/min, which means that for an injection time of 0.04 min, the volume of vapor sample injected was about 80 µL (i.e., 2 mL/min x 0.04 min x 1000 µL/mL).

The fuel samples were evaluated using a mixed hydrocarbon standard, which consisted of an equal volume mix of the normal alkanes pentane (C<sub>5</sub>) through dodecane (C<sub>12</sub>). Volumes of 1, 0.5, 0.25, and 0.1 µL of the mixed standard were placed into separate sealed chilled headspace vials and processed in the same way as for the fuel samples. Using the gas chromatographic retention times of the hydrocarbon standards, the fuel vapor chromatograms were divided into eight subsections, 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 pentane vapor density regression equation, only to calculate subsection vapor densities, which were summed to obtain total fuel vapor density. The single pentane regression equation was used instead of eight regression equations (C<sub>5</sub>-C<sub>12</sub>), since results from a related project suggested that this approach would give more consistent and accurate data.

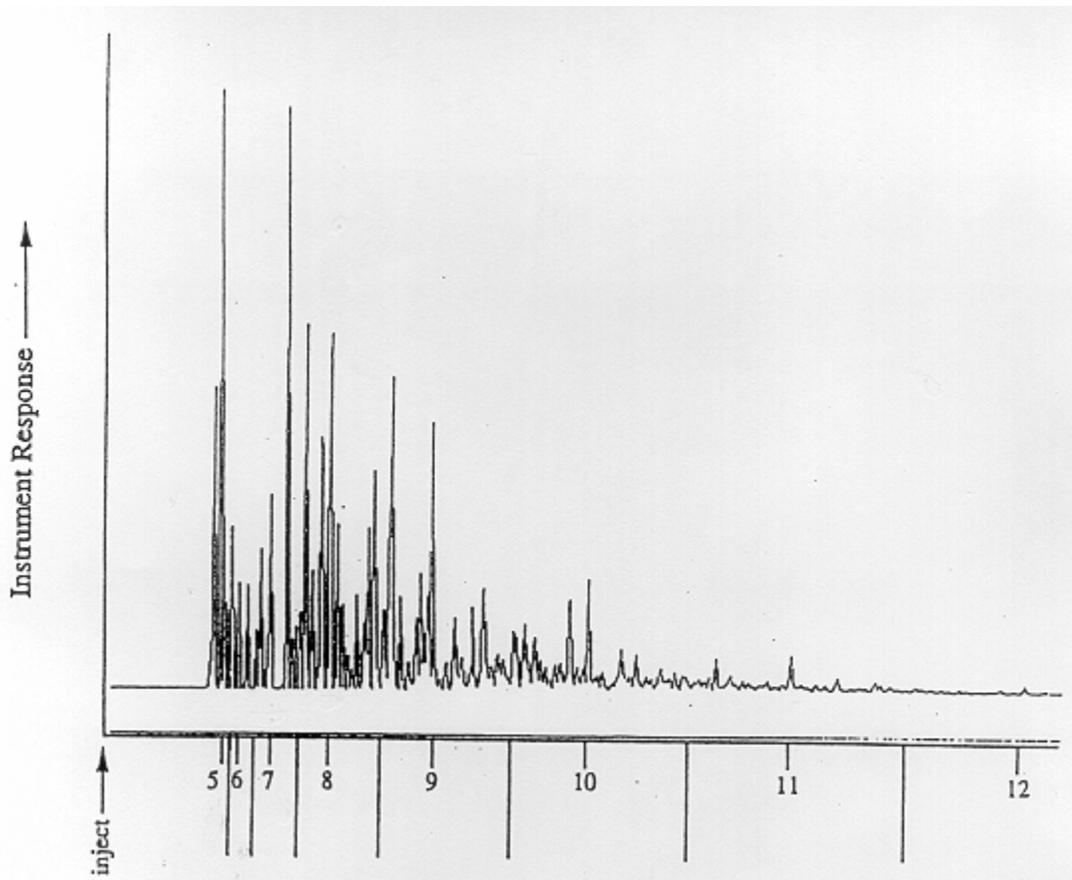


FIGURE 1. TYPICAL HEADSPACE GAS CHROMATOGRAM OF JET A VAPOR SHOWING STANDARD RETENTIONS (CARBON NUMBERS 5-12) AND SUBSECTIONS (Vertical lines)

### LIQUID FUEL METHOD.

For purposes of comparison and as a check of the vapor results, each of the 11 fuel samples was injected as the neat liquid (0.1-0.2  $\mu\text{L}$ ) onto a 60 m x 0.32 mm (i.d.) DB-1 FSOT capillary column (J&W Scientific), and each hydrocarbon component was monitored using a flame ionization detector installed in a Hewlett-Packard model 5890 Series II gas chromatograph. All samples were automatically injected using a computer-controlled enhanced autoinjector with a nanoliter adapter installed (Agilent, Wilmington, DE). The capillary column was held at 50°C for 4 minutes, programmed at a rate of 1°C/min to 250°C, where it was held for 10 minutes. Each run took about 3.6 hours to complete. Starting with eicosane (C<sub>20</sub>), and working down in carbon number, a mixed hydrocarbon standard (pentane through eicosane) was prepared by weighing each component as it was added to the mixture. The mixed standard was chromatographed under the same conditions used for the liquid fuel samples. Based on elution

times for the reference hydrocarbons, each fuel chromatogram was divided into 16 subsections, with each subsection centered approximately on its respective reference hydrocarbon (figure 2). By injecting different amounts of the standard mixture, a regression equation was generated for each fuel subsection. From these regression equations, fuel properties, such as subsection mole fraction and partial pressure, were derived. The subsection partial pressures, calculated at the fuel flash points, were used to calculate subsection mass density of the vapor.

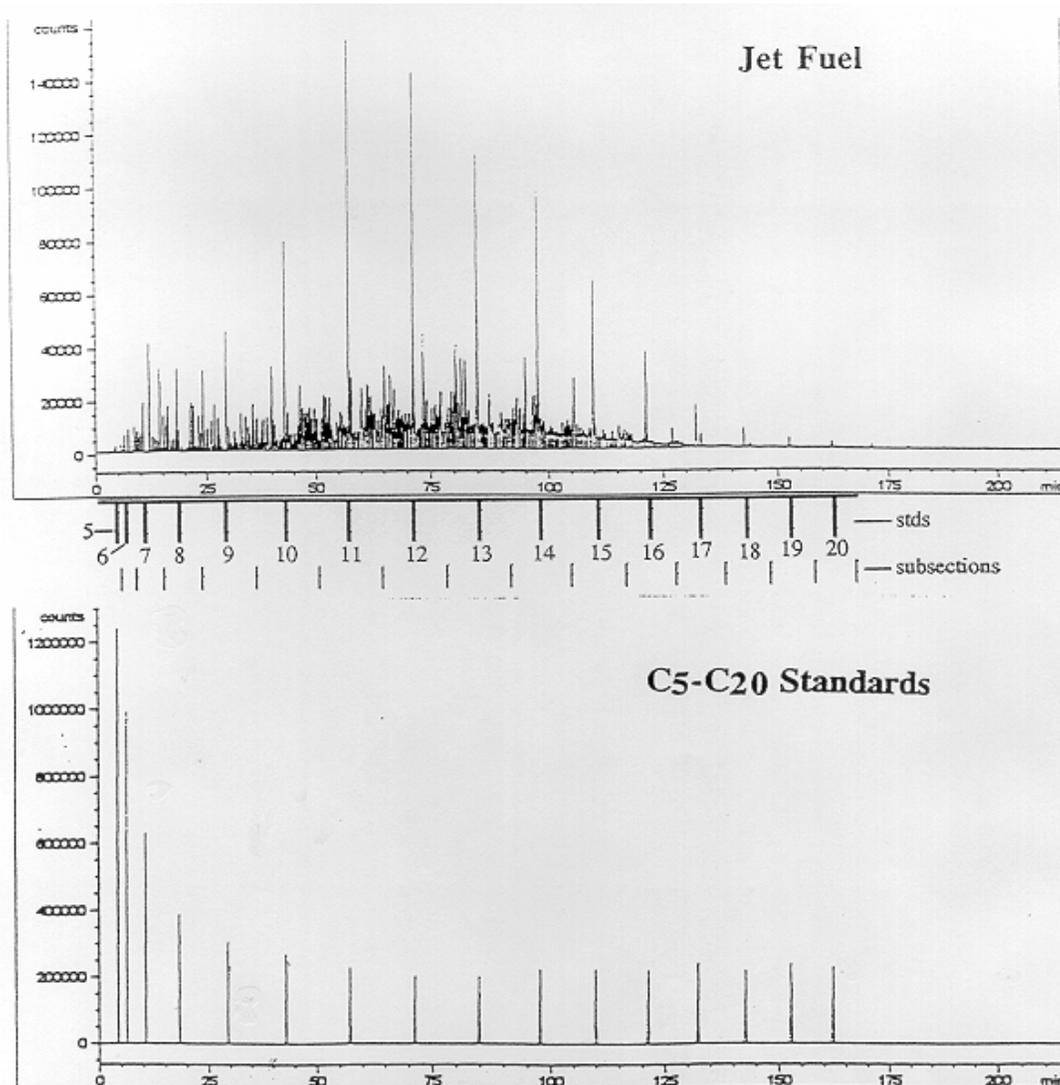


FIGURE 2. TYPICAL JET A LIQUID CHROMATOGRAM AND n-ALKANE (C<sub>5</sub>-C<sub>20</sub>) RETENTION TIMES

### DATA PROCESSING.

The raw data generated by the analytical instrumentation consisted of gas chromatographic (GC) peak areas of the individual hydrocarbon components of the fuels. Using the chromatography software, the GC peaks falling into each subsection (figures 1 and 2) were summed, reducing the number of peaks from several hundred to eight, for the vapor method, and sixteen, for the liquid

fuel method. These summed areas were then treated as individual peaks in the standard hydrocarbon regression equations to obtain eight vapor density values for the vapor method (standard regression: vapor density vs GC area) and 16 mass values for the liquid fuel method (standard regression: hydrocarbon mass vs GC area). These 16 values from the liquid fuel method were each divided by the molecular weight of the respective subsection standard hydrocarbon to give the number of moles of hydrocarbon in the liquid fuel represented by each subsection. From this, the mole fraction for each subsection was obtained and, ultimately, the vapor density above the liquid fuels, using Raoult's law and the ideal gas equation.

## RESULTS AND DISCUSSION

### HEADSPACE (VAPOR) METHOD.

Analysis using headspace sampling and 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 vapor density 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. No correction for real gas behavior is necessary as long as the total pressure in the sealed vials remains below or about 304 kPa, above which, gases become nonideal.

An important objective of this study was to use the described vapor method to determine component vapor densities and total vapor densities of the 11 samples of commercial Jet A fuel at their respective flash point temperatures. The analytical instrumentation sampled the sealed vials using a pneumatic-balanced pressure principle, which involved piercing the septum of the thermostated sample by the hollow sampling needle, pressurizing the vial, and then injecting an aliquot of the equilibrated headspace vapor onto the FSOT column using the vial pressure as the driving force.

In earlier vapor characterization projects, quantitation of the equilibrated jet fuel vapor was accomplished using eight standard regression equations (i.e., one for each of the eight fuel vapor subsections) derived from a mixture of eight normal alkanes (pentane through dodecane) (Woodrow and Seiber, 1997; Woodrow, 2000). In these studies, 1, 0.5, 0.25, and 0.1  $\mu\text{L}$  was typically added to separate headspace vials, which were heated to completely vaporize the hydrocarbon mix, leading to eight standard curves of vapor density vs GC peak area. However, results from a related project demonstrated that the use of the pentane regression equation only for subsections C<sub>5</sub>-C<sub>12</sub>, instead of all eight regression equations, will give more consistent and accurate data (Woodrow, 2000). This is a consequence of the way the headspace instrument responds to higher molecular weight (lower volatility) reference standards below, but near, their saturation vapor densities. For example, as sample temperature is lowered, higher carbon number subsections (i.e., C<sub>10</sub>-C<sub>12</sub>) will be biased toward higher vapor density values, because the

slopes of the regression equations for these subsections will decrease as the reference standards approach vapor saturation at the lower temperature. This decrease in slope can be as much as 35%-40% for dodecane, for a temperature decrease of 20°C, while for pentane, the decrease in slope is less than 4% for the same change in temperature. Of course, the assumption is that the individual components in the higher carbon number subsections are well below their saturation vapor densities, and results from other studies show this to be the case. This temperature effect on the slope of a regression equation becomes minimal for the higher molecular weight hydrocarbons at sample temperatures >60°C. Since the fuel flash point temperatures all fell below this limit, the single pentane standard regression was used to process the fuel vapor data discussed in this report.

Vapor density results for the 11 jet fuel samples are summarized in table 1, where vapor density is listed for each of the eight subsections, along with total density for each fuel. Since the headspace instrument did not allow fractional temperatures, flash point temperatures were rounded to the nearest whole value for processing the fuel samples. Determination of total fuel vapor density was fairly precise, as shown by the percent relative standard deviation (%RSD) range of 0.41-4.0 (median: 1.8). Table 2 lists dry-air density values, calculated at the rounded flash point temperatures, and the FAMR for each fuel. The FAMRs fell in the range 0.041-0.047, with an average value of 0.044 (median: 0.044) and a %RSD of 4.5.

From the vapor density values for the fuel samples, it is possible to calculate other fuel vapor properties, such as vapor pressure and average molecular weight. Table 3 lists subsection partial pressure and total vapor pressure for the fuels, and table 4 lists subsection mole percent and average molecular weight for the fuel vapor. These data can be used to compare fuels to show how the flash point is directly related to the composition of the fuel vapor, as illustrated in figure 3 for four of the test fuels. Fuel sample No. 362 (flash point = 38°C) had a hydrocarbon distribution in the vapor with a maximum at about C<sub>8</sub>. Except for the obvious light hydrocarbon spike that appeared in subsection C<sub>5</sub>, fuel sample No. 298 had a similar hydrocarbon distribution, with a maximum at about C<sub>8</sub> as well. However, the predominate C<sub>5</sub> spike in fuel sample No. 298 effectively raised its volatility (vapor pressure = 13.9 mbar, compared to 11.9 mbar for fuel sample No. 362) and lowered its flash point (30° compared to 38°C for fuel sample No. 362). At the other end of the flash point scale (58° and 59°C), fuel sample Nos. 225 and 367 had hydrocarbon distributions with maxima at about C<sub>10</sub>, with corresponding vapor pressures of 10.1 and 9.18 mbar for sample Nos. 225 and 367, respectively. Compared to fuel sample No. 367, fuel sample No. 225 had a slightly higher vapor pressure due to the relatively greater enrichment in subsections C<sub>5</sub> and C<sub>6</sub>. Similar comparisons could be made for the remaining fuels. These comparisons show that fuels enriched in the heavier, less volatile hydrocarbons had the higher flash points.

TABLE 1. SUBSECTION AND TOTAL VAPOR DENSITY FOR 11 COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (HEADSPACE [VAPOR] METHOD)

FAA No.	Flash Point (°C) <sup>a</sup>	Subsection Vapor Density, g/m <sup>3</sup>								Total g/m <sup>3</sup> ) <sup>b</sup>
		5	6	7	8	9	10	11	12	
204	49	0.198	0.288	3.94	12.0	12.8	10.2	4.99	0.939	45.4 ±1.8
211	52	1.46	3.44	6.74	9.26	10.5	9.02	4.82	1.40	46.6 ±1.1
225	58	1.11	1.20	3.37	6.74	11.4	13.3	7.90	2.05	47.1 ±1.3
270	41	2.33	2.93	8.40	12.0	13.1	7.47	2.41	0.474	49.1 ±0.2
298	30	16.1	2.91	7.81	10.8	9.94	4.94	1.35	0.123	54.0 ±0.4
344	46	2.02	2.05	5.27	9.05	12.6	11.2	4.37	0.892	47.4 ±0.6
362	38	3.12	4.26	9.80	12.4	12.6	6.89	2.17	0.337	51.6 ±0.9
366	54	0.985	1.68	5.80	8.40	10.4	10.2	6.04	1.71	45.2 ±0.8
367	59	0.515	0.816	3.39	5.91	9.03	10.2	10.4	3.69	44.0 ±0.7
389	44	1.07	2.14	6.70	14.7	16.8	8.37	2.40	0.443	52.6 ±1.4
395	52	5.90	2.46	4.45	6.46	11.1	12.8	5.25	1.30	49.7 ±1.8

<sup>a</sup> Rounded to the nearest whole value.

<sup>b</sup> Average (±SD) of three determinations.

TABLE 2. FUEL/AIR MASS RATIOS DERIVED FROM DATA OBTAINED USING THE HEADSPACE (VAPOR) METHOD

FAA Fuel No.	Flash Point (°C) <sup>a</sup>	Air Density (g/m <sup>3</sup> ) <sup>b</sup>	Fuel Vapor Density (g/m <sup>3</sup> )	Fuel/Air Mass Ratio
204	49	1095.8	45.4	0.041
211	52	1085.7	46.6	0.043
225	58	1066.0	47.1	0.044
270	41	1123.8	49.1	0.044
298	30	1164.6	54.0	0.046
344	46	1106.1	47.4	0.043
362	38	1134.6	51.6	0.045
366	54	1079.0	45.2	0.042
367	59	1062.8	44.0	0.041
389	44	1113.1	52.6	0.047
395	52	1085.7	49.7	0.046
Average:				0.044±0.002

<sup>a</sup> Rounded to the nearest whole value.

<sup>b</sup> Derived from the following expression:  $\text{Dens. (g/m}^3) = -0.86157 + 3.5313 \times 10^5 (1/T)$ , where T is the absolute temperature.

TABLE 3. SUBSECTION AND TOTAL VAPOR PRESSURE FOR 11 COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (HEADSPACE [VAPOR] METHOD)

FAA No.	Flash Point (°C)*	Subsection Partial Pressure, mbar								Total (mbar)
		5	6	7	8	9	10	11	12	
204	49	0.073	0.089	1.05	2.81	2.67	1.92	0.855	0.148	9.62
211	52	0.547	1.08	1.82	2.19	2.21	1.71	0.833	0.222	10.6
225	58	0.423	0.383	0.926	1.62	2.45	2.57	1.39	0.331	10.1
270	41	0.843	0.888	2.19	2.74	2.67	1.37	0.402	0.073	11.2
298	30	5.62	0.851	1.96	2.38	1.95	0.875	0.218	0.018	13.9
344	46	0.742	0.631	1.39	2.10	2.60	2.09	0.742	0.139	10.4
362	38	1.12	1.28	2.53	2.81	2.54	1.25	0.359	0.051	11.9
366	54	0.371	0.530	1.57	2.00	2.20	1.95	1.05	0.273	9.95
367	59	0.197	0.261	0.934	1.43	1.94	1.98	1.84	0.598	9.18
389	44	0.391	0.654	1.76	3.39	3.45	1.55	0.405	0.068	11.7
395	52	2.21	0.771	1.20	1.53	2.34	2.43	0.908	0.206	11.6

\* Rounded to the nearest whole value.

TABLE 4. SUBSECTION MOLE PERCENT AND AVERAGE MOLECULAR WEIGHT FOR 11 COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (HEADSPACE [VAPOR] METHOD)

FAA No.	Flash Point (°C)*	Subsection Mole Percent								Average MW
		5	6	7	8	9	10	11	12	
204	49	0.764	0.930	10.9	29.2	27.8	19.9	8.88	1.53	126.2
211	52	5.15	10.2	17.1	20.6	20.8	16.1	7.85	2.09	118.7
225	58	4.19	3.80	9.17	16.1	24.2	25.5	13.8	3.28	128.3
270	41	7.54	7.94	19.6	24.5	23.9	12.3	3.60	0.650	114.8
298	30	40.5	6.13	14.1	17.2	14.1	6.30	1.57	0.131	97.96
344	46	7.11	6.04	13.4	20.1	24.9	20.0	7.10	1.33	120.5
362	38	9.37	10.7	21.2	23.5	21.3	10.5	3.01	0.429	111.7
366	54	3.73	5.33	15.8	20.1	22.2	19.6	10.6	2.74	123.5
367	59	2.15	2.85	10.2	15.6	21.2	21.6	20.0	6.52	132.2
389	44	3.35	5.60	15.1	29.0	29.6	13.3	3.47	0.587	118.8
395	52	19.1	6.65	10.4	13.2	20.2	21.0	7.83	1.78	115.9

\* Rounded to the nearest whole value.

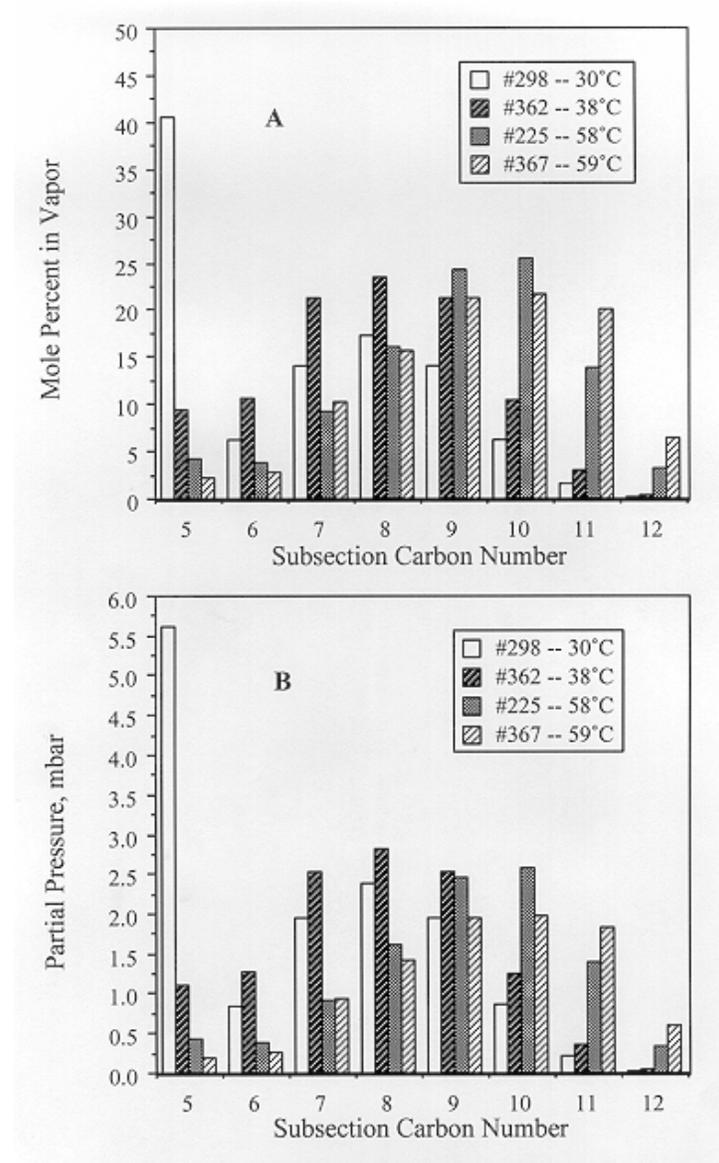


FIGURE 3. COMPARISON OF RELATIVE VAPOR DENSITY (a) AND PARTIAL PRESSURE (b) FOR 4 JET FUELS AT FLASH POINT EXTREMES

**LIQUID FUEL METHOD.**

Compared to the characterization of the fuel vapor using the headspace method, determination of the composition of the liquid fuels provided an alternative, but equivalent, way of deriving fuel properties. Figure 2 shows a typical chromatogram for liquid fuel, along with a chromatogram of the mixed hydrocarbon standard. By dividing the chromatogram into 16 subsections, each represented by a standard normal alkane, it was possible to reduce the typically 300-400+ GC peaks to 16 peaks by adding the GC peak areas in each subsection. These summed areas were then used in the standard regression equations for each subsection to calculate the equivalent hydrocarbon mass for each subsection. Using the molecular weight of each standard normal

alkane, each subsection mass was converted to moles of equivalent hydrocarbon and then to mole fraction.

Table 5 lists the subsection mole percent values for each of the 11 fuels as well as the average molecular weights for the liquid fuels. These liquid mole percent values can be used to calculate fuel vapor pressure at any given temperature. For example, table 6 lists subsection partial pressures and total vapor pressures calculated for each fuel at the exact flash point. Calculations were made for the subsections up through C<sub>16</sub> only, since standard normal alkane vapor pressures became insignificant for the higher carbon number subsections. By using the liquid subsection partial pressures, in the ideal gas equation, the molar density of the vapor above each liquid fuel was estimated at the exact flash point temperature. The results of this calculation are summarized in table 7 as subsection vapor mass density (i.e., the product of subsection molar density and the molecular weight of the standard normal alkane) and total vapor mass density for the 11 fuels. Calculation of total vapor density had a %RSD range of 0.40-1.7, with a median value of 0.63 (compare to the %RSD for the headspace method result of 0.41-4.0 (median: 1.8)). Finally, table 8 lists dry-air density values, calculated at the exact flash point temperatures, and the FAMR for each fuel. The FAMRs fell in the range 0.043-0.045, with an average value of 0.044 (median: 0.044) and a %RSD of 2.3 (compared to the average value for the headspace method of 0.044 (median: 0.044) and a %RSD of 4.5).

### COMPARING THE METHODS.

Tables 9 and 10 summarize a comparison of selected fuel vapor properties that were derived from both the headspace (vapor) and liquid fuel methods. Also included are the percent differences (%Δ) between the various property values from the two different methods. Overall, data from the two methods compared reasonably well. For example, the percent difference for the vapor density values fell in the range 0%-6.6%, with an average of 3.3% (median: 3.7%); and for the individual FAMR values, the percent difference fell in the range 0%-7.1%, with an average difference of 3.0% (median: 3.2%) (table 9). For vapor pressure, the percent difference fell in the range of 0%-8.7%, with an average difference of 4.0% (median: 3.2%); and for the average molecular weight of the fuel vapor, the percent difference range was 0%-1.7%, with an average difference of 0.92% (median: 0.85%) (table 10). This comparison indicates that the two methods provided essentially equivalent fuel property results. However, the liquid fuel method appeared to give somewhat more precise data, and the raw data from this method could be used to calculate fuel properties for any set of conditions, whereas the data obtained using the headspace (vapor) method were unique to the sample test conditions. Fuel sample No. 298 (flash point: 29.6°C) presented something of an anomaly in that the fuel property data obtained using the headspace (vapor) method appeared to be reasonable (e.g., vapor density: 54 g/m<sup>3</sup>; FAMR: 0.046 (table 2)); whereas, compared to the vapor method, the liquid fuel method considerably underestimated the properties for this fuel (e.g., vapor density: ~35 g/m<sup>3</sup>; FAMR: ~0.030). The rather prominent, high volatility component in subsection C<sub>5</sub>, for the fuel vapor (figure 3), did not seem to appear in the same subsection for the liquid method (i.e., the summed area for liquid subsection C<sub>5</sub> was almost an order of magnitude less than what would have been expected based on the vapor results). Some losses of a volatile component (e.g., propane and butane) might have occurred with the liquid analytical instrument, but it is not clear how this could have happened. Data for this fuel obtained, using the liquid fuel method, were not reported, since the difference between the results from the two methods could not be resolved by the time this report was due.

TABLE 5. SUBSECTION MOLE PERCENT AND AVERAGE MOLECULAR WEIGHT FOR 11 LIQUID COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (LIQUID FUEL METHOD)

FAA No.	Flash Point (°C) <sup>a</sup>	Subsection Mole Percent of Liquid Fuel							
		5	6	7	8	9	10	11	12
204	49.1	0.005	0.025	0.957	5.01	11.5	21.7	23.8	17.3
211	52.0	0.032	0.217	1.08	2.85	7.77	15.6	20.0	18.1
225	57.5	0.018	0.062	0.462	1.90	6.72	17.5	22.8	20.5
270	41.1	0.060	0.270	2.05	6.81	16.7	23.3	20.1	14.8
298	29.6	--	--	--	--	--	--	--	--
344	46.5	0.050	0.157	1.10	4.02	12.8	26.2	24.4	16.9
362	37.5	0.074	0.419	2.60	7.74	18.6	26.7	22.5	13.8
366	54.1	0.020	0.112	0.919	2.55	7.76	16.9	23.0	20.6
367	59.0	0.012	0.051	0.472	1.45	5.44	14.2	30.7	27.2
389	43.5	0.029	0.185	1.54	6.76	17.4	20.9	17.3	13.6
395	51.6	0.097	0.152	0.715	2.18	8.90	22.0	20.9	17.8

FAA No.	Subsection Mole Percent of Liquid Fuel								Average MW
	13	14	15	16	17	18	19	20	
204	9.84	5.37	2.95	1.11	0.421	--	--	--	157.6
211	15.2	10.5	5.49	2.10	0.819	0.130	--	--	166.6
225	16.2	9.30	3.19	1.03	0.139	0.035	0.005	0.001	164.9
270	8.94	4.40	1.72	0.561	0.143	0.019	0.008	0.001	152.0
298	--	--	--	--	--	--	--	--	-- <sup>b</sup>
344	9.08	3.90	1.15	0.198	0.021	0.006	0.002	--	153.9
362	5.11	1.62	0.567	0.110	0.003	0.001	--	--	146.7
366	14.9	7.93	3.58	1.32	0.324	0.033	0.003	0.001	163.7
367	13.5	4.94	1.51	0.343	0.047	0.006	--	--	162.7
389	10.3	6.88	3.35	1.22	0.402	0.043	--	--	155.4
395	14.6	9.47	2.80	0.363	0.013	0.001	--	--	161.6

<sup>a</sup> FP = flash point.

<sup>b</sup> Results for fuel sample No. 298 were inconclusive using the liquid fuel method.

TABLE 6. SUBSECTION PARTIAL PRESSURE AND TOTAL VAPOR PRESSURE FOR 11 COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (LIQUID FUEL METHOD)

FAA No.	Flash Point (°C) <sup>a</sup>	Subsection Partial Pressure, mbar							
		5	6	7	8	9	10	11	12
204	49.1	0.071	0.129	1.73	3.19	2.60	1.80	0.722	0.193
211	52.0	0.538	1.24	2.18	2.08	2.04	1.54	0.732	0.248
225	57.5	0.370	0.433	1.17	1.77	2.33	2.32	1.15	0.399
270	41.1	0.680	1.04	2.69	2.96	2.43	1.22	0.362	0.095
298	29.6	--	--	--	--	--	--	--	--
344	46.5	0.712	0.741	1.79	2.27	2.52	1.88	0.626	0.158
362	37.5	0.791	1.40	2.86	2.80	2.22	1.11	0.320	0.068
366	54.1	0.309	0.696	2.02	2.06	2.27	1.87	0.948	0.321
367	59.0	0.245	0.372	1.26	1.44	2.02	2.04	1.69	0.583
389	43.5	0.376	0.780	2.20	3.30	2.91	1.25	0.367	0.104
395	51.6	1.61	0.862	1.43	1.56	2.29	2.10	0.740	0.235

FAA No.	Subsection Partial Pressure, mbar				Total VP (mbar)
	13	14	15	16	
204	0.048	0.008	0.002	--	10.5
211	0.091	0.021	0.004	0.001	10.7
225	0.144	0.028	0.004	--	10.1
270	0.024	0.004	--	--	11.5
298	--	--	--	--	-- <sup>b</sup>
344	0.037	0.005	--	--	10.7
362	0.010	0.001	--	--	11.6
366	0.104	0.018	0.003	--	10.6
367	0.133	0.016	0.002	--	9.80
389	0.034	0.007	0.001	--	11.3
395	0.086	0.018	0.002	--	10.9

<sup>a</sup> FP = flash point.

<sup>b</sup> Results for sample #298 were inconclusive using the liquid fuel method.

TABLE 7. SUBSECTION AND TOTAL VAPOR DENSITY FOR 11 COMMERCIAL JET FUELS AT THEIR FLASH POINT TEMPERATURES (LIQUID FUEL METHOD)

FAA No.	Flash Point (°C) <sup>a</sup>	Subsection Vapor Density (g/m <sup>3</sup> )							
		5	6	7	8	9	10	11	12
204	49.1	0.192	0.414	6.48	13.6	12.4	9.58	4.21	1.23
211	52.0	1.44	3.95	8.10	8.80	9.66	8.10	4.23	1.56
225	57.5	0.972	1.36	4.26	7.35	10.8	12.0	6.57	2.48
270	41.1	1.97	3.44	10.1	12.9	12.0	6.58	2.18	0.619
298	29.6	--	--	--	--	--	--	--	--
344	46.5	1.93	2.40	6.75	9.76	12.2	10.0	3.69	1.02
362	37.5	2.21	4.69	11.1	12.4	11.0	6.11	1.94	0.449
366	54.1	0.956	2.21	7.48	8.60	10.7	9.74	5.44	2.01
367	59.0	0.641	1.16	4.59	5.97	9.41	10.5	9.57	3.60
389	43.5	1.03	2.55	8.39	14.3	14.2	6.75	2.18	0.670
395	51.6	4.31	2.75	5.31	6.59	10.9	11.1	4.28	1.48

FAA No.	Subsection Vapor Density (g/m <sup>3</sup> )				Total, g/m <sup>3b</sup>
	13	14	15	16	
204	0.333	0.062	0.014	0.002	48.5 ±0.2
211	0.622	0.153	0.032	0.005	46.6 ±0.3
225	0.966	0.200	0.029	0.004	47.0 ±0.3
270	0.172	0.028	0.004	--	50.0 ±0.4
298	--	--	--	--	-- <sup>c</sup>
344	0.257	0.037	0.004	--	48.0 ±0.4
362	0.075	0.008	0.001	--	50.0 ±0.3
366	0.708	0.134	0.025	0.004	48.0 ±0.3
367	0.886	0.118	0.015	0.002	46.5 ±0.8
389	0.236	0.052	0.010	0.002	50.4 ±0.2
395	0.586	0.133	0.016	0.001	47.4 ±0.3

<sup>a</sup> FP = flash point.

<sup>b</sup> Average (±SD) of 2-4 determinations.

<sup>c</sup> Results for sample #298 were inconclusive using the liquid fuel method.

TABLE 8. FUEL/AIR MASS RATIOS DERIVED FROM DATA OBTAINED USING THE LIQUID FUEL METHOD

FAA Fuel No.	Flash Point (°C)	Air Density (g/m <sup>3</sup> )*	Fuel Vapor Density (g/m <sup>3</sup> )	Fuel/Air Mass Ratio
204	49.1	1095.5	48.5	0.044
211	52.0	1085.7	46.6	0.043
225	57.5	1067.6	47.0	0.044
270	41.1	1123.4	50.0	0.044
344	46.5	1104.4	48.0	0.043
362	37.5	1136.4	50.0	0.044
366	54.1	1078.7	48.0	0.044
367	59.0	1062.8	46.5	0.044
389	43.5	1114.9	50.4	0.045
395	51.6	1087.0	47.4	0.044
Average:				0.044 ±0.001

\* Derived from the following expression:  $\text{Dens. (g/m}^3) = -0.86157 + 3.5313 \times 10^5 (1/T)$ , where T is the absolute temperature.

TABLE 9. COMPARISON OF FUEL VAPOR DENSITY AND FAMR DERIVED FROM THE HEADSPACE (VAPOR) AND LIQUID FUEL METHODS

Fuel No.	Ave. Vapor Density, g/m <sup>3</sup>			Fuel/Air Mass Ratio (FAMR)		
	HS-GC <sup>a</sup>	Liq.-GC <sup>b</sup>	%Δ	HS-GC	Liq.-GC	%Δ
204	45.4	48.5	6.6	0.041	0.044	7.1
211	46.6	46.6	-0-	0.043	0.043	-0-
225	47.1	47.0	0.21	0.044	0.044	-0-
270	49.1	50.0	1.8	0.044	0.044	-0-
344	47.4	48.0	1.2	0.043	0.043	-0-
362	51.6	50.0	3.1	0.045	0.044	2.2
366	45.2	48.0	6.0	0.042	0.044	4.6
367	44.0	46.5	5.5	0.041	0.044	7.1
389	52.6	50.4	4.3	0.047	0.045	4.3
395	49.7	47.4	4.7	0.046	0.044	4.4

<sup>a</sup> HS-GC = headspace gas chromatograph. Fuel properties were derived from vapor characterization.

<sup>b</sup> Liq.-GC: Fuel properties for the vapor were derived from liquid characterization.

TABLE 10. COMPARISON OF FUEL VAPOR PRESSURE AND AVERAGE MOLECULAR WEIGHT DERIVED FROM THE HEADSPACE (VAPOR) AND LIQUID FUEL METHODS

Fuel No.	Vapor Pressure, mbar			Ave. Molecular Weight (vapor)		
	HS-GC <sup>a</sup>	Liq.-GC <sup>b</sup>	%Δ	HS-GC	Liq.-GC	%Δ
204	9.62	10.5	8.7	126	124	1.6
211	10.6	10.7	0.94	119	118	0.84
225	10.1	10.1	-0-	128	128	-0-
270	11.2	11.5	2.6	115	114	0.87
344	10.4	10.7	2.8	120	119	0.84
362	11.9	11.6	2.6	112	111	0.90
366	9.95	10.6	6.3	124	123	0.81
367	9.18	9.80	6.5	132	131	0.76
389	11.7	11.3	3.5	119	117	1.7
395	11.6	10.9	6.2	116	117	0.86

<sup>a</sup> HS-GC = headspace gas chromatograph. Fuel properties were derived from vapor characterization.

<sup>b</sup> Liq.-GC: Fuel properties for the vapor were derived from liquid characterization.

### SUMMARY

1. The fuel-to-air mass ratio (FAMR) values were essentially constant at the fuel flash point temperatures, and the typical FAMR value at the flash point was 0.044.
2. Both the headspace (vapor) and liquid fuel methods gave results that were essentially equivalent, building confidence in the data. The liquid fuel results appeared to have better precision.
3. Using Raoult's law, the liquid fuel results can be used to calculate fuel vapor properties at any given temperature, if the saturation vapor pressures for the reference hydrocarbons at those temperatures are known. The headspace (vapor) results were unique to the fuel sample test conditions.
4. The fuel property results (i.e., hydrocarbon distribution in the vapor) from both the headspace (vapor) and liquid fuel methods can be used in a comparative way to explain the differences in fuel flash points.

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