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Application of the Advanced Distillation Curve Method to the Variability of Jet Fuels

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Supporting Information

ABSTRACT: In this paper, we report the application of the advanced distillation-curve (ADC) approach to the gas turbine fuels Jet-A, JP-8, and JP-5, in order to obtain information about the variability of these gas turbine fuels. The measurements of the ADC derived temperatures T_k and T_h provide volatility information as an approximation of the vapor−liquid equilibrium, VLE. The composition channel of the advanced distillation curve provides access to more detailed insight into the fluid behavior. Finally, we have shown how the composition channel allows the combination of thermochemical data with the temperature data of the distillation curve. The variability in distillation curves and calculated heat of combustion between jet fuels is significant. Understanding of this variability is critical information for a more effective and reliable thermophysical property modeling system.

INTRODUCTION

Jet fuels are complex mixtures of hydrocarbons derived from petroleum through refinement processes, and they contain many possible hydrocarbons ranging from six to eighteen carbons.[1] The most common commercial gas turbine fuels are Jet-A and Jet-A-1. Jet-A and Jet-A-1 are similar, with Jet-A-1 being widely available outside the U.S.A. and having a lower freeze point (−47 °C instead of −40 °C for Jet-A). Jet-A is available in the U.S.A. and is required to meet the specifications of ASTM-D1655,[2] which requires the fuel to be sampled and tested appropriately to examine the conformance to detailed requirements as to composition, volatility, fluidity, combustion, corrosion, thermal stability, contaminants, and additives.[2]

The major gas turbine fuel that is used by the United States military is JP-8 (MIL-DTL-83133),[1] a kerosene fraction that has a higher flash point than its main military predecessor, JP-4, which contained a wide cut of petroleum distillate with material from the lighter naptha fraction as well as the kerosene fraction of petroleum.[1] JP-8 is very similar to Jet-A-1, with the major differences being in the additive package. JP-8 contains an icing inhibitor, corrosion/lubricity enhancer, and antistatic additive.[3] Aboard aircraft carriers, the only aviation kerosene used is JP-5 (MIL-DTL-5624U), which has a somewhat higher flash point than Jet-A or JP-8 (desirable for safety considerations). Its higher cost restricts its use to the specialized fire control needs of aircraft carriers.

Commercial and military gas turbine fuels are purchased under specifications defining the physical properties of the products. These specifications permit broad variation in chemical composition to ensure an adequate supply. An important way to understand these variations within fuel types is to analyze the volatility by measurements of the distillation curves. In earlier work, the method and apparatus for determining advanced distillation curves (ADCs) was described, and the resulting information has proven to be especially applicable to the characterization of fuels.[4−13] This method offers significant improvements over previous approaches, such as ASTM D-86, and can be applied to any complex fluid.[8−15] It features (1) a composition-explicit data channel for each distillate fraction (for both qualitative and quantitative analyses), (2) temperature measurements that are true thermodynamic state points that can be modeled with an equation of state (EOS), (3) temperature, volume, and pressure measurements of low uncertainty suitable for EOS development, (4) consistency with a century of historical data, (5) an assessment of the energy content of each distillate fraction, (6) trace chemical analysis of each distillate

Table 1. Initial Boiling Behavior of Jet Fuels

fuel	onset (°C)	sustained (°C)	vapor rise (°C)
Jet-A LMO	174.7	180.6	192.0
Jet-A WBU	179.3	183.4	187.6
Jet-A DEN	175.2	182.8	190.6
Jet-A FNL	174.9	181.6	194.7
Jet-A APA	137.3	187.9	189.7
Jet-A 3602	150.9	183.6	191.0
Jet-A 3638	148.4	176.9	184.2
Jet-A 4597	162.9	175.4	187.5
Jet-A 4598	191.8	196.8	203.3
Jet-A 4599	177.5	182.3	188.5
Jet-A 4600	126.8	178.5	177.6
Jet-A 4658	139.9	185.6	190.5
Jet-A 4877	148.3	191.6	193.1
Jet-A 5237	149.5	190.8	193.8
Jet-A 5245	143.5	195.1	199.0
Jet-A 5677	154.4	192.5	196.5
Jet-A 5916	135.9	191.7	198.0
Jet-A 6407	143.2	179.8	182.5
JP-8 4751	147.3	174.5	190.6
JP-8 6169	171.6	176.1	184.7
JP-8 3773	157.6	178.4	189.7
JP-5 4810	178.3	195.6	200.1

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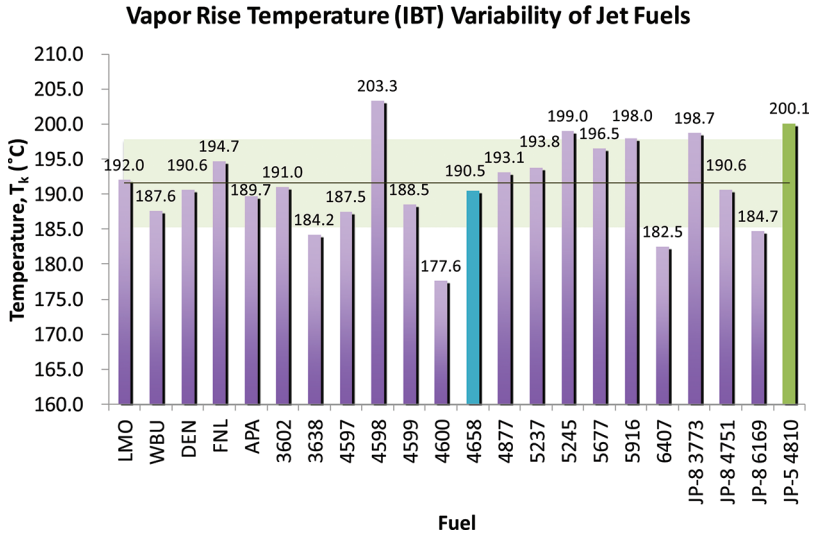

Figure 1. Vapor rise temperatures of measured jet fuels. The samples are Jet-A unless specifically labeled as JP-8 or JP-5. The line is the average vapor rise temperature and the shaded area is one standard deviation. The uncertainties are discussed in the text. 4658 is shaded blue because it is a composite of five Jet-A fuels, and JP-5 4810 is shaded green because it is formulated to have a higher flash point than Jet-A or JP-8.

fraction, and (7) corrosivity assessment of each distillate fraction.[8−15]

In this paper, we report the application of the advanced distillation-curve approach to the gas turbine fuels Jet-A, JP-8, and JP-5, in order to assess the variability of gas turbine fuels.[16]

EXPERIMENTAL SECTION

Five samples of Jet-A were obtained from airports located in Colorado. Thirteen samples of Jet-A, three samples of JP-8, and one sample of JP-5, representing different processing lots, were obtained from the Fuels Branch of the Air Force Research Laboratory (AFRL, Wright Patterson Air Force Base). The Jet-A samples from Colorado are designated with three letter airport codes, the other Jet-A samples are designated numerically, and the JP-8 and JP-5 samples are designated with JP-8 and JP-5 followed by a numerical identifier. The sample Jet-A-4658 is a composite of five batches of Jet-A (from multiple manufacturers), which was mixed in approximately equal volumes to provide an "average" Jet-A. The samples were maintained in sealed containers, and no solidification or phase separation was noted during storage.

With the exception of JP-8-3773, which had previously been analyzed,[17,18] the general composition of each sample of gas turbine fuel was studied by a gas chromatography (GC) method (30 m capillary column of 5% phenyl/95% dimethyl polysiloxane, with a thickness of 0.25 μm) with mass spectrometry (MS) detection and flame ion detection (FID).[19,20] The GC analysis of all samples was performed by passing a He carrier gas at 55.2 kPa (8 psi, gauge) through the column while undergoing sample-independent temperature programming: the column was held for 4 min at 60 °C, and then the temperature was increased to 275 °C at a rate of 20 °C/min. After elution of all sample components, the column was held at 275 °C for 4 min, ensuring complete removal of the solvent (acetone) and trace contaminants from the column prior to the next sample injection. MS was used with the aid of the NIST/EPA mass spectral database,[20,21] following column separation to provide compositional information by identification of peaks in the resulting chromatogram. These analytical results (compositions and relative quantities of components) are consistent with our knowledge of each fuel. We will note later in this paper that these analyses are also consistent with the results from the composition-explicit data channel of the ADC. The components, which make up 1% or more of the neat fuel samples, can be seen in the Supporting Information, Table S1.

ADC Measurements. The ADC apparatus and procedure have been described in much detail in previous papers;[8,9,12,13,22−24] thus, only a brief description (as it applies to this study) will be given here. For each measurement, 200 mL of fuel was placed in a boiling flask. The thermocouples were then inserted into the proper locations to monitor (a) the kettle temperature (T_k), the temperature in the fluid, and (b) the head temperature (T_h), the temperature at the bottom of the takeoff position in the distillation head. In terms of significance, T_k is a thermodynamically consistent bubble point temperature, while T_h approximates what might be obtained from the classical distillation measurement procedure. We note that a direct comparison of the ADC and ASTM D-86 has been done for prototype diesel fuels.[25] Enclosure heating was then commenced with a model-predictive temperature controller.[11] The heating profile was designed to be of similar shape to that of the distillation curve, but it leads the distillation curve by approximately 20 °C. As heating progressed, the volume of the distilled liquid was measured in a level-stabilized receiver. Measurements of the kettle and head temperatures were recorded at specific distillate volume fractions to construct the distillation curve. For distillate fraction sample analysis, approximately 7 μL sample aliquots were collected at the receiver adapter hammock. As we have noted in previous work, the angle of the hammock minimized entrainment or hysteresis among the samples.[26] Over the course of the work, at least three distillation curves were measured for each fuel sample. The temperatures for each distillate fraction were averaged over the three separate measurements, and the standard deviations were also determined.

Because the measurements of the distillation curves were performed at an elevation of approximately 1655 m above sea level at local ambient atmospheric pressure (typically 83 kPa, measured with an electronic barometer with an uncertainty of 0.003 kPa), temperature readings were corrected for what should be obtained at standard atmospheric pressure. The pressure adjustments were performed with the modified Sydney Young equation, in which the constant term was assigned a value of 0.000109.[24,27,28] This value corresponds to a *n*-alkane carbon chain of 12, which is a reasonable approximation for the composition of gas turbine fuel.

RESULTS AND DISCUSSION

Initial Boiling Temperatures (IBTs). During the initial heating of each sample in the distillation flask, the fluid behavior was observed. Direct observation through the bore scope ports allowed for the measurement of the onset of the boiling behavior for each fluid. Typically, during the earlier stages of measurements, the first bubbles will appear intermittently and are rather small. These bubbles cease if the stirrer is stopped momentarily. The temperature at which this is observed is called the onset

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Table 2. Representative Distillation Curve Data (Given as the Average of Three Distillation Curves) for Jet-A, JP-8, and JP-5[a]

distillate vol. frac. (%)	Jet-A LMO 82.70 kPa		Jet-A WBU 82.66 kPa		Jet-A DIA 82.55 kPa	
	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)
5	197.3	182.1	197.2	186.3	194.0	171.5
10	200.4	185.0	198.9	190.8	197.1	179.8
15	203.4	187.9	200.7	193.8	200.0	186.5
20	206.3	192.7	202.3	195.5	202.8	188.7
25	209.1	196.5	204.0	197.2	205.5	191.0
30	211.5	195.9	205.7	199.1	208.5	192.4
35	214.0	198.7	207.5	201.1	211.0	196.0
40	216.5	206.9	209.3	202.9	213.6	198.1
45	218.5	208.6	211.3	205.0	216.4	200.1
50	221.4	211.7	213.3	207.3	219.8	207.8
55	224.1	215.1	215.4	209.3	222.9	211.2
60	226.8	218.9	217.4	211.4	225.9	216.5
65	230.0	222.4	220.3	214.1	230.1	222.3
70	233.4	227.0	222.5	216.3	233.8	226.4
75	237.3	231.4	225.4	219.1	238.2	231.4
80	240.8	235.2	228.4	221.8	242.9	234.9
85	245.7	242.1	232.2	224.6	248.6	241.4

distillate vol. frac. (%)	Jet-A FNL 82.70 kPa		Jet-A APA 82.66 kPa		Jet-A 3602 82.55 kPa	
	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)
5	197.6	190.6	191.3	184.2	191.0	179.3
10	199.7	192.7	191.7	181.5	194.8	186.7
15	201.5	193.7	192.6	184.8	197.7	189.9
20	203.2	190.6	194.0	188.4	200.7	194.7
25	204.8	193.9	195.7	190.7	203.5	196.9
30	206.7	197.1	197.0	192.2	206.4	198.7
35	208.5	200.0	198.4	194.2	209.7	199.2
40	210.5	203.0	199.9	195.9	212.1	201.5
45	212.8	206.8	201.6	199.0	214.8	204.5
50	215.3	207.2	203.3	201.5	217.3	206.4
55	217.6	212.6	205.0	203.9	220.1	208.8
60	219.5	214.6	206.9	206.3	222.5	213.6
65	223.7	217.4	208.9	208.9	225.1	213.7
70	226.9	224.4	211.2	212.3	227.9	218.4
75	230.8	226.6	213.5	215.6	230.7	223.2
80	234.9	231.4	216.9	219.0	233.9	226.4
85	240.4	239.7	219.9	226.0	237.9	225.6

distillate vol. frac. (%)	Jet-A 3638 82.70 kPa		Jet-A 4597 82.66 kPa		Jet-A 4598 82.55 kPa	
	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)
5	184.2	179.9	191.8	173.3	208.0	185.0
10	186.8	184.2	194.9	180.8	210.3	190.2
15	188.7	187.0	198.0	185.7	213.3	196.8
20	191.1	185.8	200.4	190.9	216.2	201.4
25	192.9	189.5	202.8	194.6	219.3	204.5
30	194.9	191.6	205.8	196.4	222.5	206.6
35	196.6	193.9	207.9	197.9	225.3	207.2
40	198.5	196.0	210.2	199.3	229.1	214.2
45	200.3	197.9	212.6	203.2	232.4	219.6
50	202.1	199.8	215.7	205.8	236.4	226.6
55	204.0	202.4	218.0	208.6	239.3	230.0
60	205.9	204.0	220.8	211.3	243.3	233.2
65	208.0	205.1	224.3	241.9	248.3	236.9
70	210.5	207.6	227.4	223.0	252.3	239.3
75	213.6	210.6	231.3	226.8	256.7	243.5
80	216.2	210.2	235.5	233.6	260.8	250.0
85	219.4	215.3	240.4	235.8	266.9	256.0

distillate vol. frac. (%)	Jet-A 4599 82.70 kPa		Jet-A 4600 82.66 kPa		Jet-A 4658 82.55 kPa	
	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)
5	196.0	175.0	184.8	167.6	190.5	174.7
10	200.0	178.0	188.7	171.8	195.4	183.3
15	203.7	184.4	192.5	176.8	198.5	187.0
20	207.1	187.9	196.3	184.8	201.5	189.1
25	210.4	194.4	200.1	189.0	204.7	190.6
30	213.2	198.7	203.7	192.8	208.1	192.8
35	216.2	201.5	207.5	198.5	211.3	194.6
40	219.3	206.0	211.5	201.3	214.3	199.1
45	222.1	208.8	215.5	206.2	217.6	202.6
50	225.5	212.1	219.7	210.0	220.7	205.4
55	228.8	216.3	224.0	214.4	224.2	208.6
60	232.3	220.0	228.6	218.3	227.6	212.4
65	236.5	224.8	233.3	223.4	231.2	214.9
70	240.6	229.5	238.4	225.9	234.7	216.6
75	245.5	234.6	244.1	230.3	239.4	218.7
80	250.5	243.0	250.2	237.2	243.3	220.8
85	256.2	247.8	257.6	241.4	247.9	224.1

distillate vol. frac. (%)	Jet-A 4877 82.70 kPa		Jet-A 5237 82.66 kPa		Jet-A 5245 82.55 kPa	
	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)	T_k (°C)	T_h (°C)
5	195.5	181.1	195.4	172.3	202.1	194.4
10	197.0	186.6	196.7	184.6	204.2	193.5
15	198.2	188.6	198.2	187.1	206.4	191.5
20	199.8	191.1	199.7	190.5	209.0	197.4

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Table 2. continued

distillate vol. frac. (%)	Jet-A 4877 82.70 kPa T_k (°C)	Jet-A 4877 82.70 kPa T_h (°C)	Jet-A 5237 82.66 kPa T_k (°C)	Jet-A 5237 82.66 kPa T_h (°C)	Jet-A 5245 82.55 kPa T_k (°C)	Jet-A 5245 82.55 kPa T_h (°C)
25	201.2	193.1	201.2	193.0	211.5	202.6
30	202.4	195.0	202.5	194.2	213.8	205.7
35	203.8	197.8	204.0	196.4	216.2	209.8
40	205.3	198.7	205.5	198.4	218.8	212.6
45	206.9	201.3	207.4	199.5	221.6	215.1
50	208.5	203.0	209.0	202.2	224.2	216.9
55	210.2	205.4	210.8	204.1	226.8	221.4
60	212.2	206.5	212.8	207.4	229.8	225.2
65	214.3	210.6	214.9	209.9	232.9	227.8
70	216.6	212.5	217.2	212.7	236.3	231.8
75	219.4	216.2	219.9	215.4	239.9	236.7
80	222.6	220.0	223.2	218.2	244.0	242.1
85	226.8	221.9	226.8	225.7	249.3	249.0

distillate vol. frac. (%)	Jet-A 5677 82.70 kPa T_k (°C)	Jet-A 5677 82.70 kPa T_h (°C)	Jet-A 5916 82.66 kPa T_k (°C)	Jet-A 5916 82.66 kPa T_h (°C)	Jet-A 6407 82.55 kPa T_k (°C)	Jet-A 6407 82.55 kPa T_h (°C)
5	199.6	191.9	202.2	189.4	183.8	180.2
10	202.2	179.8	205.0	189.3	184.7	173.2
15	205.0	183.6	207.6	191.7	185.8	175.3
20	207.9	188.9	210.8	194.4	186.9	176.8
25	210.8	198.5	213.7	198.8	188.1	179.6
30	213.5	203.7	216.0	202.8	189.2	179.9
35	216.1	206.3	218.5	206.3	190.4	182.6
40	219.2	210.6	221.0	211.9	191.8	183.7
45	222.2	214.2	223.4	213.2	193.5	185.6
50	225.3	217.9	225.9	215.5	195.1	187.4
55	228.5	221.7	228.3	218.8	196.8	190.1
60	234.5	225.5	231.0	222.2	198.8	192.1
65	235.6	229.9	233.7	224.5	201.3	194.9
70	239.4	234.4	236.7	227.8	204.1	198.4
75	243.6	239.6	240.1	202.9	207.5	202.4
80	248.5	245.2	244.0	236.7	211.9	207.2
85	254.2	252.0	248.6	243.8	217.6	213.4

distillate vol. frac. (%)	JP-8 4571 82.70 kPa T_k (°C)	JP-8 4571 82.70 kPa T_h (°C)	JP-8 6169 82.66 kPa T_k (°C)	JP-8 6169 82.66 kPa T_h (°C)	JP-8 3773 82.55 kPa T_k (°C)	JP-8 3773 82.55 kPa T_h (°C)
5	195.0	174.4	189.2	165.0	192.5	184.1
10	197.9	180.5	192.1	169.6	194.2	186.7
15	200.7	185.5	195.0	174.7	196.3	188.7
20	203.3	190.1	197.7	179.8	198.1	190.8
25	206.2	193.6	200.2	182.1	200.6	193.3
30	208.6	196.0	202.7	186.4	203.0	195.9
35	211.2	197.9	205.3	189.2	205.2	198.6
40	213.9	199.8	208.4	191.9	207.8	201.4
45	216.5	202.4	211.0	194.9	210.5	204.4
50	219.6	205.9	214.0	198.7	213.2	207.4
55	222.2	208.4	217.2	201.1	216.3	210.6
60	225.2	211.9	220.5	204.5	219.7	214.2
65	228.8	216.9	224.5	209.4	223.4	217.9
70	232.1	221.9	228.7	212.8	227.4	221.8
75	235.9	225.1	233.2	218.9	231.6	226.2
80	238.5	231.5	238.3	223.9	236.9	231.3
85	241.3	233.5	244.3	230.8	242.8	236.3

distillate vol. frac. (%)	JP-5 4810 82.70 kPa T_k (°C)	JP-5 4810 82.70 kPa T_h (°C)
5	202.5	192.1
10	204.1	195.6
15	206.0	198.3
20	207.7	200.7
25	209.6	203.0
30	211.4	204.7
35	213.3	206.9
40	215.9	208.9
45	218.0	210.7
50	220.2	212.7
55	223.3	215.6
60	225.9	217.9
65	229.4	220.2
70	233.4	222.3
75	236.4	225.3
80	240.5	229.8
85	248.1	232.8

[a]The uncertainties are discussed in the text. These temperatures have been adjusted to 1 atm with the Sydney Young equation; the experimental atmospheric pressures are provided to allow recovery of the actual measure temperatures.

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temperature. Sustained bubbling, which occurs subsequent to onset, is characterized by larger, more vigorous bubbles and is still observed when the stirring is briefly stopped. Finally, vapor is observed to rise into the distillation head, causing an immediate response on the T_h thermocouple. This temperature, called the vapor rise temperature, has been shown to be the IBT of the fluid. Furthermore, this temperature is of low uncertainty and thermodynamically consistent and can be modeled theoretically with an EOS.[29,30]

The initial temperature observations of each gas turbine fuel are summarized in Table 1. These values are the average of three separate measurements. The uncertainty (with a coverage factor $k = 2$)[31] of these measurements has been discussed in detail in previous papers and is approximately 2 °C in the onset and sustained bubbling temperatures and approximately 0.3 °C in the vapor rise temperature.[12] Figure 1 shows the vapor rise temperature for the fuel samples with the line being the average of the vapor rise temperatures and the shaded area being one standard deviation. The lowest vapor rise temperature was found for Jet-A-4600 at 179.6 °C and the highest vapor rise temperature was found for Jet-A-4598 at 203.3 °C. This 23.7 °C temperature span demonstrates the wide degree of composition differences normal in commercial jet fuels. It is interesting to note that although JP-5 does not have the highest initial boiling temperature, it is clearly at the high end for IBT and is likely to be so consistently. Our data do not imply otherwise, but JP-5 appears to be within the volatility specifications for Jet-A and JP-8.

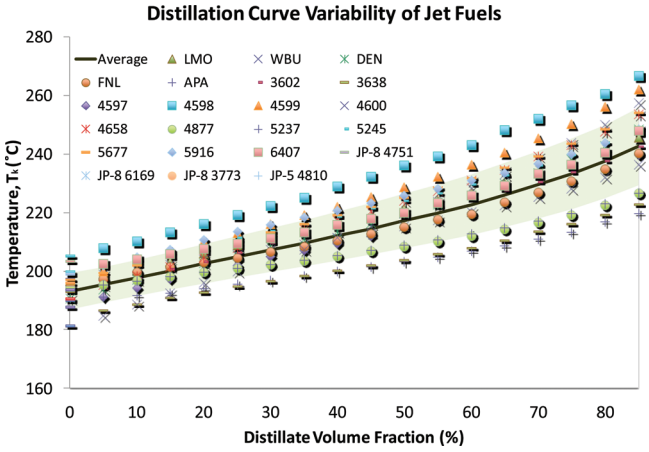

Figure 2. Distillation curves for measured jet fuels. The samples are Jet-A unless specifically labeled as JP-8 or JP-5. The line is the average of the distillation curve temperatures and the shaded area is one standard deviation. The uncertainties are discussed in the text. The hash marks on the *y*-axis are the temperatures when the first drop of distillate enters the calibrated receiver.

Distillation Curves. The distillation curve data, presented in both T_k and T_h, for all of the aviation fuels studied in this work are

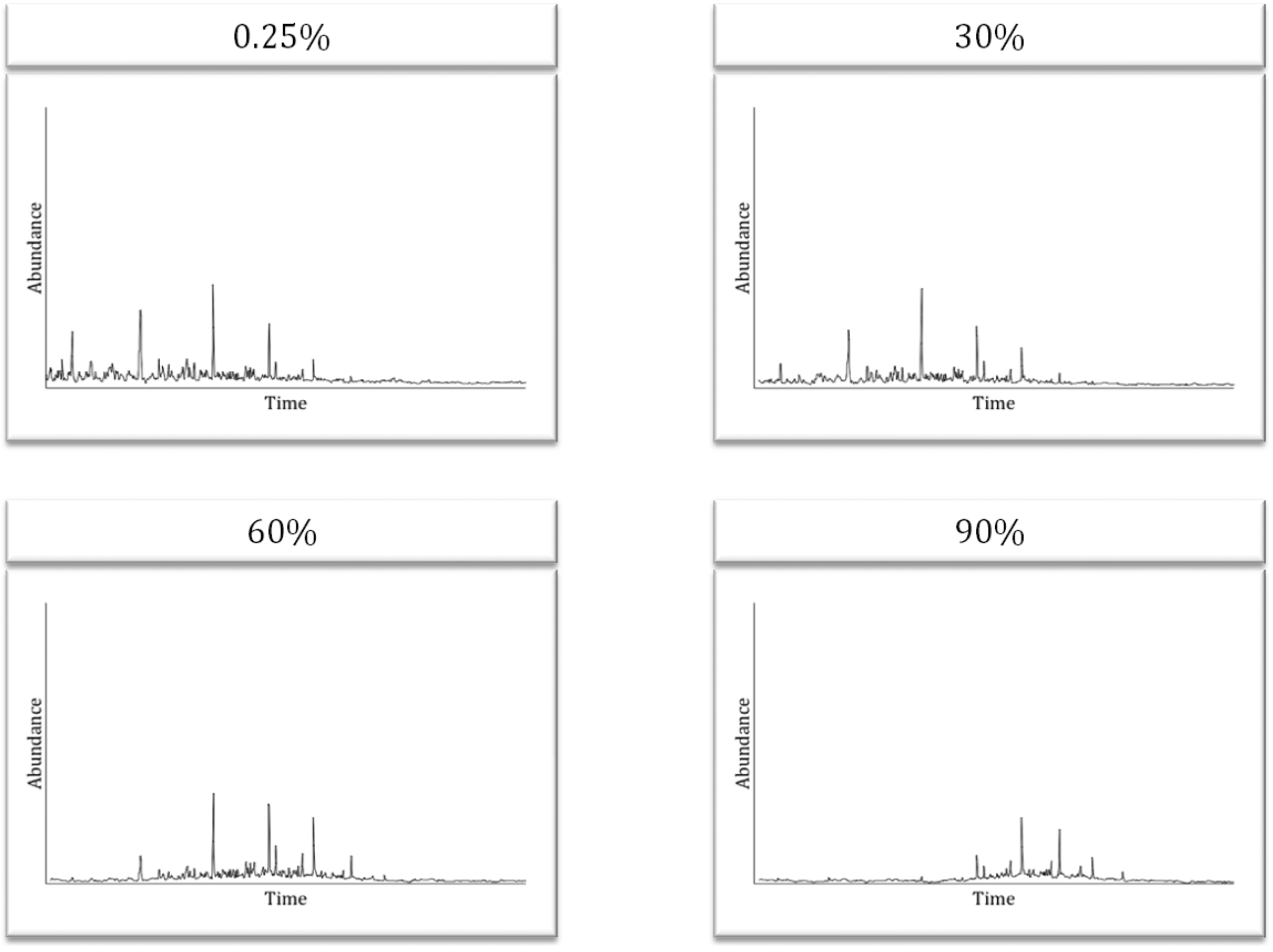

Figure 3. GC-MS chromatograms of the 0.25, 30, 60, and 90% distillate fractions of the Jet-A FNL sample.

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Table 3. Aliphatic Hydrocarbon Family Types Resulting from the ASTM D-2789 Analysis Performed on the Neat Samples of the Jet Fuels

sample	paraffins (%)	monocycloparaffins (%)	dicycloparaffins (%)	alkylbenzenes (%)	indanes and tetralins (%)	naphthalene (%)
LMO	39.7	28.6	11.7	12.3	4.5	3.3
WBU	32.5	25.5	11.8	20.1	7.2	2.9
DEN	35.6	27.6	12.7	15.1	5.5	3.5
FNL	33.3	26.3	12.1	19	6.3	3
APA	32.9	25.9	11.3	21.4	6.2	2.2
3602	29.1	25.7	13.3	20.5	8.7	2.8
3638	39.9	26	11.1	15.7	4	3.4
4597	40	25	10	17.2	4.1	3.7
4598	31.3	28.5	13.4	16.3	7.1	3.4
4599	34.8	23.7	11.6	17.7	8.5	3.7
4600	34.3	23.3	10.9	19.7	8.2	3.6
4658	38.5	24.7	10.2	16.9	6.4	3.3
4877	38.2	21.3	8.4	23	6.9	2.1
5237	39.2	21.3	8.2	22.4	6.7	2.1
5245	38.9	25.2	10.5	16.4	7	2
5677	38.7	24.9	10.9	16.4	7.2	1.9
5916	32	26.2	14	16	7.6	4.1
6407	33.2	25.4	14.6	19.4	6	1.4
JP-8 4751	38.6	23.3	9.3	17.9	7.6	3.3
JP-8 6169	41.3	24.6	9.8	16	5.1	3.3
JP-8 3773	38.9	27.2	10.6	15.2	4.8	3.3
JP-5 4810	36.9	28.4	13.2	13.3	4.4	3.7

provided in Table 2. Graphically, the distillation curves (T_k) can be seen in Figure 2, with the line representing the average of the distillation curves, the shaded area being one standard deviation, and the hash marks representing the temperature corresponding to the first drop in the calibrated receiver. The distillation data for Jet-A 3602, Jet-A 3638, Jet-A 4658, and JP-8 3773 have been reported previously but are included here for completeness.[13,18] The T_k data are true thermodynamic state points, while the T_h data allow for a comparison to historical measurements. The data in this table were found to be highly reproducible and comparable to the repeatability achieved in our previous work with the ADC.

The distillation curves for all the jet fuels appear to be of subtle sigmoid shape, which is expected for a complex fluid with many components distributed over a large range of relative molecular mass. There was no indication of the presence of azeotropic behavior in any of the jet fuels samples. If the fuels showed azeotropic characteristics, one would observe the convergence of T_k and T_h, and this is not seen in any of the jet fuels measured.[2,32] The first drop temperatures have a spread that is approximately 25 °C, and the spread at the 80% fraction is approximately 45 °C. The distillation curve of Jet-A 4810 has higher temperatures for each distillate volume fraction. Jet-A APA and JP-8 3638 have the lowest temperatures for most distillate volume fractions. This behavior was previously noted for Jet-A 3638 and is related to a relatively high concentration of light components.[13] It should be noted that JP-5, which is specified for its high flash point, does not have the highest temperature distillation curve, although it certainly is at the high range in temperature.

As we have mentioned, it is possible to use the T_h measured by the ADC method as a means of comparison with the historical data obtained by ASTM D-86. Such historical data can be obtained from the *Petroleum Quality Information System 2009 Annual Report*, the last year for which the comparison is published.[33] In that compilation, the temperature of the 10% recovered fraction is the only temperature on the distillation curve proper that is not only reported but which falls within a given specification. The other temperature specified by the range is the final boiling temperature, which is not measured by the ADC, and which is off the distillation curve, in any case. While not exactly equivalent, the T_h, given by the ADC at this distillate volume fraction, can be compared with this range reported for 2009. The 10% recovered temperatures, expressed in our work as T_h, fall within the range of minimum and maximum compiled for JP-8 and JP-5 for 2009. The reported 10% recovered for JP-8 had a maximum of 205 °C and a minimum of 151.2 °C. Our data had a 10% recovered temperature at 169.9 °C for JP-8 6169 and 180.5 for JP-8 4751. The reported 10% recovered for JP-5 had a maximum of 204 °C and a minimum of 167 °C. Our data had a 10% recovered temperature of 195.6 for JP-5. The reported 10% recovered for Jet-A had a maximum of 176 °C and a minimum of 172 °C. Our data had a minimum of 171.8 °C but a maximum value of 193.5 °C, a wider range than what is reported for 2009.

Distillation Composition. While the gross examination of the distillation curves is instructive and valuable for many design purposes, the composition channel of the advanced approach can provide an even greater understanding and information content. One can sample and examine the individual fractions as they emerge from the condenser. Sampling was performed by withdrawing approximately 7 μL aliquots of distillate (at various distillate volume fractions) and diluting the aliquot in a known mass (~1 mL) of acetone as a solvent. This fluid was chosen as a solvent because it had a short retention time and did not interfere with any of the GC peaks of the distillate fractions. Each of these fractions was analyzed by GC with FID and MS method using the same column and oven temperature program as that described for the neat sample analysis. To quantify the compositional mole fractions in the distillate cuts, calibration on the FID was performed with octane.

To help visualize the composition progression during the distillation, chromatograms for Jet-A FNL are presented in Figure 3. For each chromatogram, the x-axis represents the

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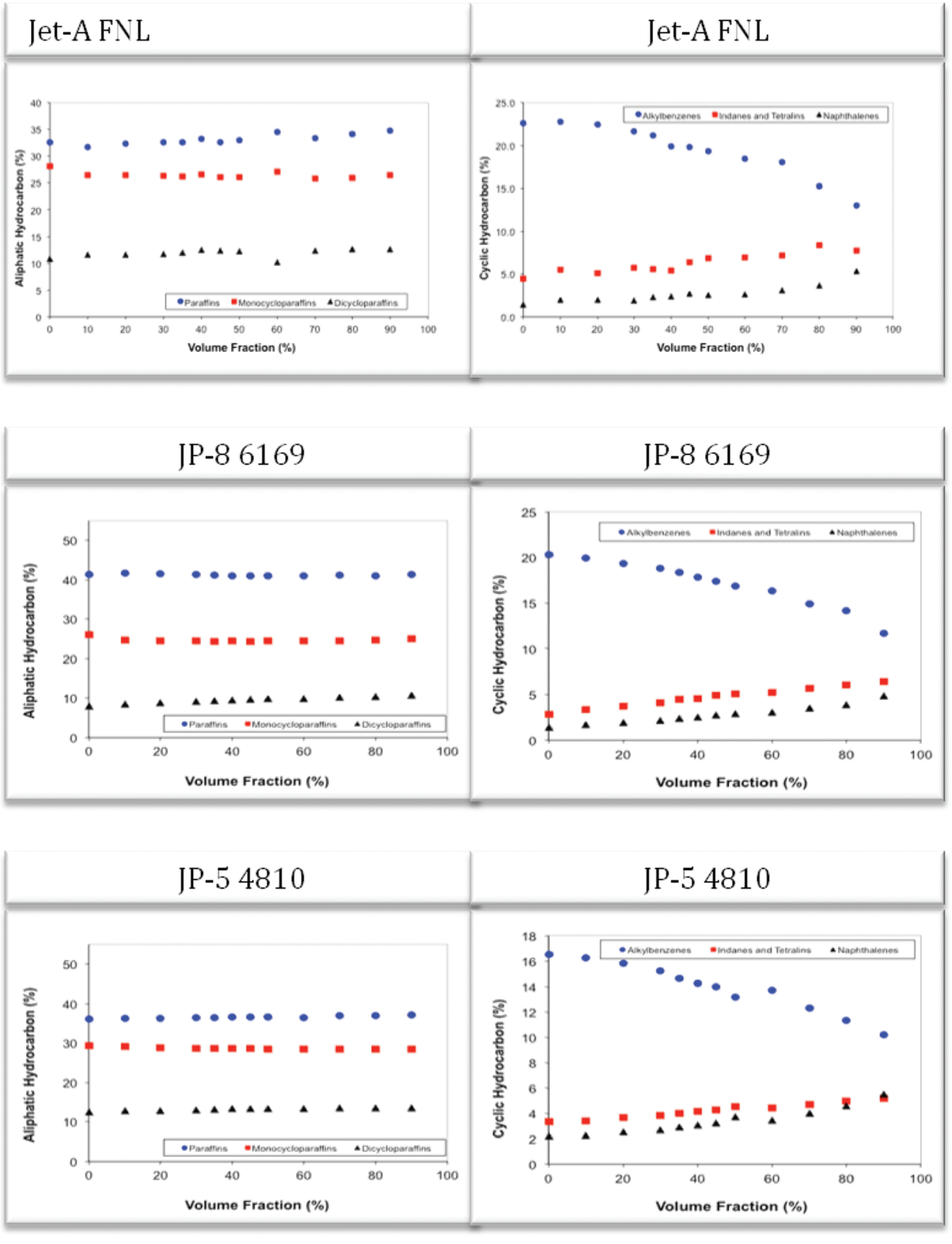

Figure 4. Plots of the hydrocarbon family types resulting from the ASTM D-2789 analysis performed on (a) Jet-A FNL, (b) JP-8 6168, and (c) JP-5 4810.

retention time in minutes, and the *y*-axis indicates the abundance presented in arbitrary units of area counts (voltage slices). It should be noted that the solvent (acetone) peak appeared at the beginning of the chromatogram and is not shown, having been electronically removed. In this series of chromatograms, one can see the gradual decrease of the lighter, more volatile components, and the increase of the heavier, less volatile components as the distillations progressed. Figure 3 illustrates just one fraction-by-fraction analysis strategy that can be applied to the composition-explicit data channel. It is possible to use any analytical technique that is applicable.

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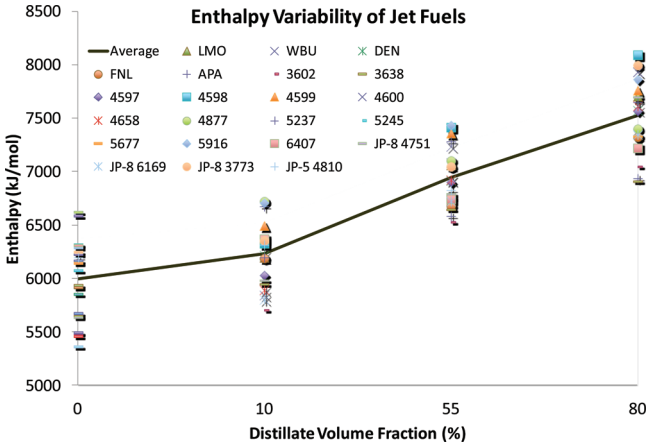

Figure 5. Energy content, presented as the composite enthalpy of combustion, $-\Delta H_c$ (kJ/mol), as a function of the distillate volume fraction for jet fuels. The line runs through the average enthalpy at the distillate volume fractions. The uncertainties are discussed in the text.

Hydrocarbon Classification. Another analytical technique that complements the above analyses examines the jet fuel samples for hydrocarbon types by use of a mass spectrometric classification method similar to that summarized in ASTM D-2789.[34] In this method, one uses MS (or GC-MS) to characterize hydrocarbon samples into six types. The six types or families include the following: paraffins, monocycloparaffins, dicycloparaffins, alkylbenzenes (arenes or aromatics), indanes and tetralins (grouped as one classification), and naphthalenes. Although the method is specified only for application to low olefinic gasoline and has significant limitations, it is of practical relevance to many complex fluid analyses and is often applied to gas turbine fuels, rocket propellants, and missile fuels.[35] The uncertainty of this method and the potential pitfalls were discussed earlier.[12] Once again, the sample solutions were prepared from ~7 μL aliquots of emergent distillate that were withdrawn from the sampling adapter at specified volume fractions and added to a vial containing a known mass of solvent (acetone). For the hydrocarbon-type analysis of the distillate fraction samples, 1 μL of these solutions was injected into the GC-MS. Because of this consistent injection volume, no corrections were needed for sample volume.

The results of the hydrocarbon classification for the neat jet fuel samples can be seen in Table 3. The fuels had an average of 36.3% paraffins with a standard deviation of 3.45%, an average of 25.4% monocycloparafins with a standard deviation of 2.0%, an average of 11.3% dicycloparaffins with a standard deviation of 1.7%, an average of 17.6% alkylbenzenes with a standard deviation of 2.8%, an average of 6.4% indanes and tetralins with a standard deviation of 1.4%, and an average of 3.0% naphthalene with a standard deviation of 0.7%. The graphical results of the hydrocarbon classification for Jet-A FNL, JP-8 6168, and JP-5 4810 are presented in Figure 4. In the jet fuels, there is no clear change in the composition of the distillate fraction with respect to the concentration of the aliphatic hydrocarbons during the distillations. One can observe a change in the alkylbenzenes, indanes and tetralins, and naphthalenes. The percentage of alkylbenzenes decreases significantly during the distillation and the percentage of indanes and tetralins, and naphthalenes increase somewhat toward the end of the distillation. The changes in composition with the distillate volume fraction for all of the jet fuels studied followed similar trends but are not presented here.

Distillate Fraction Energy Content. As we have demonstrated previously, it is possible to add thermochemical information to the distillation curve when the composition channel of data is used on specific distillate fractions.[12,13,22,23] This is done by calculating a composite enthalpy of combustion based on the enthalpy of combustion of individual (pure)

Table 4. Energy content, as $-\Delta H_c$ (kJ/mol), as a function of the Distillate Fraction for Jet Fuels[a]

	composite enthalpy of combustion (kJ/mol)				
distillate vol. frac. (%)	0.03%	10%	55%	80%	neat
Jet-A LMO	5937 (296.8)	6197 (309.8)	7060 (353.0)	7703 (385.2)	7134 (356.7)
Jet-A WBU	6222 (311.1)	6329 (316.4)	6783 (339.1)	7365 (368.3)	6964 (348.2)
Jet-A DEN	5853 (292.7)	6218 (310.9)	6913 (345.6)	7576 (378.8)	7008 (350.4)
Jet-A FNL	5914 (295.7)	6188 (309.4)	6684 (334.2)	7323 (366.2)	6753 (337.7)
Jet-A APA	6162 (308.1)	6197 (309.8)	6580 (329.0)	6936 (346.8)	6654 (332.7)
Jet-A 3602	5481 (274.0)	5702 (285.1)	6531 (326.5)	7046 (352.3)	5880 (294.0)
Jet-A 3638	5653 (282.6)	5945 (297.2)	6646 (332.3)	6909 (345.4)	6677 (333.8)
Jet-A 4597	5488 (274.4)	6030 (301.5)	6902 (345.1)	7563 (378.2)	7012 (350.6)
Jet-A 4598	6075 (303.7)	6329 (316.4)	7415 (370.8)	8089 (404.4)	7279 (364.0)
Jet-A 4599	6141 (307.0)	6493 (324.6)	7361 (368.1)	7760 (388.0)	7640 (382.0)
Jet-A 4600	5673 (283.6)	5847 (292.3)	7083 (354.1)	7930 (396.5)	7221 (361.0)
Jet-A 4658	5455 (272.8)	5893 (294.7)	6926 (346.3)	7613 (380.7)	6733 (336.6)
Jet-A 4877	6621 (331.0)	6719 (335.9)	7104 (355.2)	7401 (370.1)	7109 (355.4)
Jet-A 5237	683 (329.2)	6672 (333.6)	7285 (364.2)	7650 (382.5)	7118 (355.9)
Jet-A 5245	6558 (327.9)	6825 (341.4)	7781 (389.0)	8070 (403.5)	7736 (386.8)
Jet-A 5677	6468 (323.4)	6665 (333.2)	7646 (382.3)	8428 (421.4)	7666 (383.3)
Jet-A 5916	6289 (314.5)	6706 (335.3)	7437 (371.8)	7863 (393.2)	7493 (374.6)
Jet-A 6407	6307 (315.4)	6369 (318.4)	6743 (337.2)	7221 (361.0)	6863 (343.2)
JP-8 4751	5638 (281.9)	5978 (298.9)	6793 (339.7)	7698 (384.9)	6889 (344.4)
JP-8 6169	5357 (267.8)	5818 (290.9)	6724 (336.2)	7345 (367.3)	6719 (335.9)
JP-8 3773	6243 (312.1)	6353 (317.7)	7047 (352.4)	7993 (399.7)	
JP-5 4810	61693 (309.6)	6313 (315.6)	6823 (341.2)	7342 (367.1)	7017 (350.8)

[a]The uncertainties are discussed the text and are provided in parentheses.

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Table 5. Energy Content on a Mass Basis, as $-\Delta H_c$ (kJ/g), as a Function of the Distillate Fraction for Jet Fuels[a]

	composite enthalpy of combustion (kJ/mol)				
distillate vol. frac. (%)	0.03%	10%	55%	80%	neat
LMO	43.5 (2.2)	43.6 (2.2)	43.7 (2.2)	43.5 (2.2)	44.0 (2.2)
WBU	43.2 (2.2)	43.1 (2.2)	43.0 (2.2)	43.4 (2.2)	43.2 (2.2)
DEN	43.4 (2.2)	43.4 (2.2)	43.2 (2.2)	43.1 (2.2)	43.3 (2.2)
FNL	43.2 (2.2)	43.3 (2.2)	43.2 (2.2)	43.2 (2.2)	43.2 (2.2)
APA	43.5 (2.2)	43.4 (2.2)	43.2 (2.2)	43.4 (2.2)	43.3 (2.2)
3602	42.9 (2.1)	42.9 (2.1)	42.9 (2.1)	43.0 (2.2)	43.2 (2.2)
3638	43.2 (2.2)	43.4 (2.2)	43.6 (2.2)	43.5 (2.2)	43.5 (2.2)
4597	43.7 (2.2)	43.5 (2.2)	43.5 (2.2)	43.7 (2.2)	43.6 (2.2)
4598	43.5 (2.2)	43.4 (2.2)	43.5 (2.2)	43.8 (2.2)	43.7 (2.2)
4599	43.0 (2.1)	42.9 (2.1)	43.1 (2.2)	43.0 (2.1)	43.4 (2.2)
4600	42.7 (2.1)	42.6 (2.1)	42.7 (2.1)	42.9 (2.1)	42.9 (2.1)
4658	43.2 (2.2)	43.2 (2.2)	43.4 (2.2)	43.1 (2.2)	43.2 (2.2)
4877	42.9 (2.1)	42.9 (2.1)	42.9 (2.1)	42.9 (2.1)	42.9 (2.1)
5237	43.2 (2.2)	43.2 (2.2)	43.3 (2.2)	43.3 (2.2)	42.9 (2.1)
5245	43.0 (2.2)	43.0 (2.2)	43.6 (2.2)	43.7 (2.2)	43.5 (2.2)
5677	43.2 (2.2)	43.2 (2.2)	43.2 (2.2)	42.9 (2.1)	43.2 (2.2)
5916	42.9 (2.1)	42.9 (2.1)	43.0 (2.2)	42.9 (2.1)	43.0 (2.2)
6407	42.9 (2.1)	42.6 (2.1)	42.9 (2.1)	43.4 (2.2)	43.0 (2.2)
JP-8 4751	43.3 (2.2)	43.1 (2.2)	43.4 (2.2)	43.6 (2.2)	43.5 (2.2)
JP-8 6169	43.2 (2.2)	43.2 (2.2)	43.4 (2.2)	43.4 (2.2)	43.3 (2.2)
JP-8 3773	43.8 (2.2)	43.8 (2.2)	43.9 (2.2)	41.2 (2.1)	
JP-5 4810	43.1 (2.2)	43.1 (2.2)	43.2 (2.2)	43.2 (2.2)	43.1 (2.2)

[a]The uncertainties are discussed the text and are provided in parentheses.

Table 6. Energy Content on a Volume Basis, as $-\Delta H_c$ (kJ/mL), as a Function of the Distillate Fraction for Jet Fuels[a]

	composite enthalpy of combustion (kJ/mL)				
distillate vol. frac. (%)	0.03%	10%	55%	80%	neat
LMO	34.1 (1.7)	34.2 (1.7)	35.6 (1.8)	36.7 (1.8)	35.5 (1.8)
WBU	34.6 (1.7)	34.8 (1.7)	35.8 (1.8)	36.7 (1.8)	35.3 (1.8)
DEN	34.0 (1.7)	34.5 (1.7)	35.8 (1.8)	36.8 (1.8)	35.5 (1.8)
FNL	34.6 (1.7)	34.8 (1.7)	35.8 (1.8)	36.3 (1.8)	35.9 (1.8)
APA	34.6 (1.7)	35.7 (1.8)	35.7 (1.8)	36.3 (1.8)	35.6 (1.8)
3602	34.2 (1.7)	34.7 (1.7)	36.21 (1.8)	36.9 (1.8)	34.42 (1.7)
3638	33.9 (1.7)	34.0 (1.7)	34.9 (1.7)	35.4 (1.8)	35.0 (1.7)
4597	33.4 (1.7)	34.2 (1.7)	35.9 (1.8)	36.5 (1.8)	35.5 (1.8)
4598	34.1 (1.7)	34.7 (1.7)	36.6 (1.8)	37.5 (1.9)	36.1 (1.8)
4599	35.1 (1.8)	35.6 (1.8)	38.0 (1.9)	38.6 (1.9)	36.6 (1.8)
4600	34.9 (1.7)	35.3 (1.8)	37.0 (1.8)	37.8 (1.8)	36.7 (1.8)
4658	33.8 (1.7)	34.6 (1.7)	36.3 (1.8)	36.7 (1.8)	35.4 (1.8)
4877	36.3 (1.8)	36.4 (1.8)	36.9 (1.8)	37.1 (1.9)	36.6 (1.8)
5237	35.5 (1.8)	35.6 (1.8)	36.4 (1.8)	36.9 (1.8)	37.3 (1.8)
5245	36.2 (1.8)	36.7 (1.8)	37.2 (1.9)	36.9 (1.8)	36.7 (1.8)
5677	35.2 (1.8)	35.5 (1.8)	36.4 (1.8)	36.1 (1.8)	36.0 (1.8)
5916	35.3 (1.8)	36.0 (1.8)	36.9 (1.8)	37.8 (1.8)	36.8 (1.8)
6407	36.4 (1.8)	36.4 (1.8)	36.7 (1.8)	37.5 (1.8)	36.8 (1.8)
JP-8 4751	33.3 (1.7)	34.0 (1.7)	35.4 (1.8)	36.9 (1.8)	35.1 (1.8)
JP-8 6169	33.7 (1.7)	34.1 (1.7)	35.3 (1.8)	35.8 (1.8)	35.0 (1.8)
JP-8 3773	32.6 (1.6)	32.5 (1.6)	32.7 (1.8)	31.2 (1.6)	
JP-5 4810	35.5 (1.8)	35.8 (1.8)	36.4 (1.8)	36.6 (1.8)	36.7 (1.8)

[a]The uncertainties are discussed the text and are provided in parentheses.

components of a distillate fraction, and the measured mole fractions of those components. The enthalpy of combustion of the individual (pure) components is taken from a reliable database compilation.[36] Uncertainty in this calculation has been attributed to a number of sources[12,13] including (1) the neglect of the enthalpy of mixing, (2) the uncertainty in the individual (pure component) enthalpy of combustion as tabulated in the database, (3) the uncertainty in the measured mole fraction, (4) the uncertainty posed by very closely related isomers that cannot be resolved by the analytical protocol, (5) the uncertainty introduced by neglecting components present at very low concentrations (that is, uncertainty associated with the chosen area cutoff), (6) the uncertainty introduced by a complete misidentification of a component, (7) the uncertainty in quantitation

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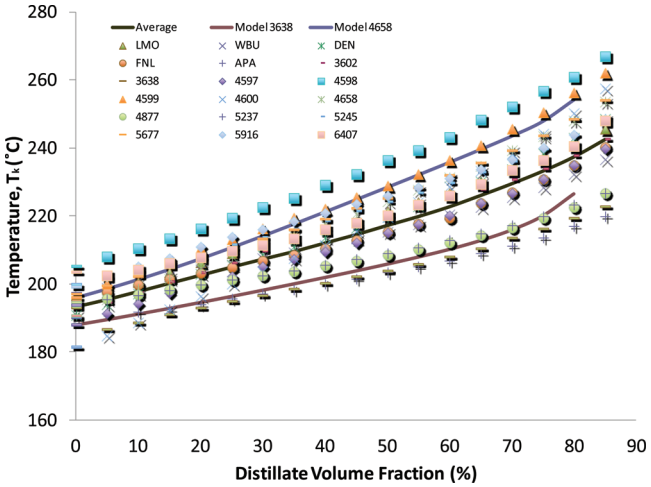

Figure 6. Distillation curves for measured Jet-A fuels. The green line is the average of the distillation curve temperatures, the purple line is the model from 4658, and the red line is the model from 3638. The hash marks on the *y*-axis are the temperatures when the first drop of distillate enters the calibrated receiver. The uncertainties are discussed in the text.

introduced by eluting peaks that are poorly resolved, and (8) the uncertainty introduced when experimental data for the pure component enthalpy of combustion are unavailable (and the Cardozo equivalent chain model must be used).[37] On the basis of the uncertainty sources listed above and the samples being investigated, a 5% uncertainty was ascribed to the calculations reported in this work.

Figure 5 shows the molar enthalpy of combustion as a function of the distillate fraction for each of the jet fuels, with a line running through the average enthalpy of combustion for the distillate volume fractions. The enthalpies with the uncertainties can be seen in Tables 4, 5, and 6. The molar enthalpy of combustion increases with distillate fraction as the concentration of longer *n*-alkanes increases in the later distillate fractions, and roughly corresponds to the variation in distillation curves. The average enthalpy ranges from 5995 kJ/mol for the first drop of distillate to 7525 kJ/mol for the 80% fraction, with a spread of approximately 1200 kJ/mol at each distillate cut. As shown in Tables 5 and 6, the enthalpies by mass and volume for all distillate cuts and fuels are very similar.

Thermophysical Property Modeling. Previous work has been done on modeling the thermophysical properties (density, sound speed, viscosity, thermal conductivity, and volatility) of Jet-A.[16] The samples used for the development of the property models were Jet-A 3638 and the composite Jet-A 4658. Figure 6 shows the distillation curves of the Jet-A fuels with lines drawn for the average of the distillation curve and the two models. The models are able to capture the volatility behavior of the two fuels very precisely, predicting values within a degree of the measured data. The volatilities of Jet-A 3638 and Jet-A 4658 differ significantly; at the end of the distillation, they are approximately 30 °C apart. Nevertheless, even with this wide range, the models do not encompass the entire range variability of Jet-A fuel volatilities studied. While it was obvious that a model based on a single fuel was not sufficient to describe all the jet fuels, before this work, we did not have sufficient evidence of the magnitude of this problem. This work therefore assists progress to be made toward developing a model that will characterize the jet fuels in terms of compositionally sensitive properties that can be used to "tune" the calculations.[16,29,30,38,39] Such properties might include selected points on the distillation curve and viscosities.

CONCLUSIONS

In this paper, we have reported the application of an improved method of distillation-curve measurement as applied to a number of jet fuels. The measurements of the temperatures T_k and T_h have a lower overall uncertainty than those of earlier methods and allow conclusions to be drawn about the fluid behavior. The composition channel of information provides access to more detailed insight into the fluid behavior. Finally, we have shown how the composition channel allows the combination of thermochemical data with the temperature data of the distillation curve. This provides an explicit measure of the energy content of each fraction. A comparison of a number of jet fuel samples allows us to better understand the variability in commercial jet fuel, which may in the future lead to a more comprehensive modeling system. A model based on a single fuel sample is not sufficient to represent the variability observed in Jet-A fuels. Future work will utilize the data presented here in order to develop a methodology to represent the fuels as a single model that will characterize the fuels in terms of compositionally sensitive properties that can be used to "tune" the calculation.

ASSOCIATED CONTENT

Supporting Information

Table S1: Major components found in neat samples of jet fuels. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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NOMENCLATURE

LMO = Vance Brand Airport, Longmont, CO
WBU = Boulder Municipal Airport, Boulder, CO
APA = Denver Centennial Airport, Denver, CO
DIA = Denver International Airport, Denver, CO
FNL = Fort Collins Municipal Airport, Fort Collins, CO

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