Comparison of Heat Capacity Measurements of Alternative and Conventional Aviation Fuels*

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Intended for submission to *Int. J. Thermophys.*

Date of this version: June 24, 2022

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Abstract

Isobaric specific heat capacities were measured for nine separate aviation turbine fuel samples. The nine samples span the range of fuel types available, including four conventional petroleumderived fuels, three synthetic fuels derived from the Fischer-Tropsch process, and two renewable fuels derived from biomass feedstocks. All measurements were made using modulated differential scanning calorimetry over the combined temperature range of (223 to 442) K. Experimental data, including an assessment of the associated expanded uncertainties, have been reported. Additionally, measurement results for the nine fuels were compared with one another and with available literature data and existing surrogate mixture models.

Keywords

Aviation fuels; Differential scanning calorimetry; Isobaric specific heat capacity; Renewable fuels; Synthetic fuels; Temperature dependence

1. Introduction

According to the International Civil Aviation Organization (ICAO), the world's airlines carried 4.3 billion passengers in 2018; this represents a 6.4% increase over 2017 [1]. Those numbers are expected to keep increasing, along with fuel costs and consumption. Consequently, improving efficiencies and securing stable fuel supplies are critical industry objectives [2]. Realizing these objectives could also potentially help the industry achieve its goal of environmental sustainability. In 2015, civil aviation consumed approximately 160 million tons of fuel, resulting in approximately 506 million tons of carbon dioxide (CO_2) emissions; a number that represents approximately 2% of global anthropogenic carbon emissions [3]. In 2008, the International Air Transport Association (IATA) committed to the goals of an average improvement in fuel efficiency of 1.5% per year through 2020, carbon neutral growth from 2020, and a 50% reduction in CO_2 emissions relative to 2005 levels by the year 2050 [4]. Both the ICAO Group on International Aviation and Climate Change (GIACC) [5] and the Federal Aviation Administration (FAA) [6] have agreed to similar goals. Given that improvements in operational and equipment efficiencies alone are not expected to be sufficient to meet carbon neutral growth targets [3], the pursuit of sustainable fuels is critical [7-10].

Jet fuels are complex mixtures made up of hundreds of different hydrocarbons; they predominantly consist of paraffins, and the relative abundance of paraffin type (normal, iso, and cyclic) varies depending on both the crude oil source and the particular refining process utilized [11]. Since jet fuels from different sources are often blended within an aircraft fuel tank, it is essential that all fuels meet the same technical specifications. Jet A and Jet A-1 are the most commonly used commercial aviation fuels, with Jet A being primarily used in the United States (US). The primary differences between the two fuels are their freeze point (233 K for Jet A vs 226

K for Jet A-1) and the fact that Jet A-1 contains a static dissipater additive [12]. Both fuels are covered under ASTM D1655, which sets requirements for composition, volatility, density, viscosity, thermal stability, materials compatibility, etc. [13].

To date, significant progress has been made in the pursuit of alternative aviation fuels. A number of possible options have been identified including synthetic fuels derived via a Fischer-Tropsch (FT) process from coal or natural gas and renewable fuels derived via a wide range of processes from multiple biomass feedstocks (e.g., vegetable oils, waste grease, algae, etc.) [7, 14]. Currently there are seven conversion processes for sustainable aviation fuel (SAF) production that have been approved under ASTM D7566 [15], thereby certifying the resulting fuels for commercial use as blends with conventional fuels. The seven approved processes are: FT synthesized paraffinic kerosene (FT-SPK), hydroprocessed esters and fatty acids SPK (HEFA-SPK), synthesized isoparaffins from hydroprocessed fermented sugars (SIP), SPK plus aromatics (SPK/A), alcohol-to-jet SPK (ATJ) for both isobutanol and ethanol, catalytic hydrothermolysis jet (CHJ), and SPK from bioderived hydroprocessed hydrocarbons, esters, and fatty acids (HC-HEFA SPK) [15]. This list could grow as additional process development is ongoing [16]. Furthermore, more than 180,000 commercial flights have been completed using conventional fuel that has been blended with SAF and there are currently seven airports regularly distributing SAF [3, 17]. Although these milestones represent a significant increase in the development and use of SAF over the last decade, large capital investments and significant policy developments are required to produce sustainable fuels in large enough quantities to make the realization of their full emissions reduction potential possible [3, 18].

A variety of factors, including feedstock availability and processing costs, ultimately determines the commercial viability of a particular alternative fuel. But more importantly, the strict quality controls surrounding aviation fuels, along with the relatively long life of a commercial jet,

necessitates that any potential alternative fuel be drop-in ready. In other words, an ideal fuel candidate would exhibit properties that would allow it to be blended with, or completely replace, existing petroleum-based fuels, without requiring modifications of the aircraft fuel system or fuel distribution network [19-22]. Important fuel properties to consider include density, thermal stability, volatility, viscosity, and heat capacity; heat capacity measurements are described in this work.

The specific heat capacity of a substance is the amount of heat-energy that must be added to one unit of mass to produce a unit change in temperature. Petroleum refinery operations and related processes require knowledge of heat capacity data over a wide range of temperatures. For example, specific heat capacity data are instrumental to the design of plant equipment, as well as to process decisions related to issues such as prolonged storage or low temperature operability. In fuel system analyses for aviation turbine engines, where the fuel is being used as a coolant, specific heat capacity data are required for heat transfer calculations. Furthermore, heat capacity can be used to evaluate other basic thermodynamic properties of a fuel. In this work, we report measurements of isobaric specific heat capacity for nine aviation fuels, including four conventional and five alternative fuels. Measurement results for six additional conventional turbine fuel samples can be found in Fortin and Bruno [23].

2. Materials and Methods

2.1 Aviation Fuel Samples

Nine samples of aviation turbine fuels, representing both conventional and alternative fuel sources, were provided by the Air Force Research Laboratory (AFRL) Propulsion Directorate at Wright-Patterson Air Force Base. For many of these nine samples, the heat capacity data presented

here complements more extensive research efforts at NIST examining the chemical and thermophysical properties of aviation fuels [24-37].

Four of the nine samples represent conventional, petroleum-based aviation turbine fuel. These include one sample each of Jet A (POSF 4658), Jet A-1 (POSF 4877), JP-8 (POSF 4751), and JP-5 (POSF 5095). The number in parentheses is the AFRL identification number, which identifies specific fuel batches. In the US, Jet A is the most commonly used commercial aviation fuel. To be eligible for sale, it must comply with the requirements detailed in ASTM D1655 [13]. This standard is primarily a performance specification since a significant degree of compositional variability is expected among fuels as a result of differences in crude sources and refining processes [13]. The sample measured in this work, Jet A (POSF 4658), is a composite mixture of several available batches of Jet A and was intended to be representative of an "average" Jet A sample. As was previously mentioned, Jet A-1 is the most common commercial aviation fuel used outside the US. It is governed by the same fuel specification as Jet A; the primary differences between the two fuels are their freeze point and the inclusion of a static dissipater additive in Jet A-1 [13]. JP-8 was first introduced at US Air Force (USAF) bases in the late 1970s and it remains the primary fuel used by the US military today, not only for aviation but for use in government diesel fueled ground vehicles as well [38]. JP-8 complies with the MIL-DTL-83133 fuel specification; it is very similar to Jet A-1 but, in addition to a static dissipator, it also contains additives to inhibit corrosion and icing [39]. Finally, JP-5 was developed in 1952 by the US Navy and remains in use today [38]. JP-5 has a higher flash point than JP-8 (333 K vs. 311 K) [39, 40], making it more suitable for use aboard aircraft carriers where fire risks are especially dire.

Three of the nine samples represent FT-SPK, which is produced by first generating a synthesis gas of primarily carbon monoxide and hydrogen from the feedstock (e.g., coal, natural gas, or biomass), and then catalytically converting the synthesis gas, via a series of chemical

reactions, to liquid fuel [41]. The first, S-8 (POSF 5018), is derived from natural gas [42]. It was developed for the USAF as a synthetic substitute for JP-8 and has been certified for use in 50/50 blends with JP-8 in B-52 aircraft [39, 42]. The second, S-5 (POSF 4705) is also derived from natural gas. It was developed as a synthetic substitute for JP-5 and conforms to most of the MIL-DTL-5624 [40] fuel specifications except for the minimum density requirement [43]. The final fuel sample, designated IPK (POSF 5642), is derived from coal [42]. It is approved for commercial use in blends of up to 50% with conventional fuels [15] and has been in use at O. R. Tambo International Airport in Johannesburg, South Africa, since 1999 [42].

The final two aviation turbine fuel samples are derived from two different bio-derived oil feedstocks. Since hydrodeoxygenation and hydroprocessing are required for fuel production, these fuels are often referred to as either hydrotreated renewable jet (HRJ) fuels or HEFA-SPK. HRJ Camelina (POSF 6152) is derived from the seeds of Camelina sativa, which is a broadleaf flowering plant in the Brassicaceae family [44]. The seed's relatively high lipid content (30% to 40% by weight) [45], as well as the crop's ability to grow well on marginal land and to tolerate drought stress conditions [46], make it attractive as a potential energy crop. Additionally, camelina's specific fatty acid profile lends itself to easier conversion into aviation fuel compared to other oilseed crops such as canola [45]. In fact, camelina derived jet fuels have been used in blends during test flights on multiple commercial and military aircraft since 2009 [47]. HRJ Tallow (POSF 6308) is derived from residual animal fats from the meat-processing industry. The comparatively low cost, as well as the possibility of reducing environmental impacts otherwise associated with their disposal, make the productive use of such feedstocks an attractive option [10]. Additionally, it is estimated that approximately five million tons of residual animal fats are produced worldwide on an annual basis; this, combined with the estimated 25 million tons of used cooking oil produced annually worldwide, is equivalent to approximately 10% of the global

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aviation fuel production in 2016 [10]. As of 2016, jet fuels derived from animal fats have been used in blends during test flights on Lufthansa's A-321 and on NASA's DC-8 [47].

The chemical composition of each of the nine fuel samples was determined by gaschromatography-mass spectrometry (GC-MS). Jet A, Jet A-1, JP-8, IPK, and HRJ Camelina were analyzed as part of earlier research efforts and the corresponding experimental details can be found in the literature [31, 32, 34]. The remaining four samples (JP-5, S-8, S-5, and HRJ Tallow) were analyzed as part of this work using the same methodology as was used for the others. Experimental details can be found in the Supplemental Information, along with tables containing the major components identified for each of the four newly-analyzed fuel samples (see Tables S1–S4 in the Supplemental Information). The previously reported [31, 32, 34] compositional analysis results for the other five fuels are shown in Tables S5–S9 for reference. In each of these tables (Tables S1–S9), chemical names and corresponding CAS registry numbers are listed, sorted by the uncalibrated chromatographic peak area. Only components with peak areas of \geq 1% are listed; for each of the nine fuels those listed components account for approximately 42% to 80% of the total measured chromatographic peak area. Tables S1 through S9 indicate that all nine fuel samples are primarily composed of linear and branched alkanes.

A mass spectral fragment classification method based on ASTM Method D-2789 [48] can be utilized to categorize hydrocarbon samples into six families: paraffins (P), monocycloparaffins (MCP), dicycloparaffins (DCP), alkylbenzenes (AB), indanes and tetralins (I&T), and naphthalenes (N). It should be noted that ASTM Method D-2789 is specified for low olefinic gasoline and, therefore, suffers from significant limitations, but can still be effective for comparing related fluids [49]. The hydrocarbon classification analysis results for Jet A, Jet A-1, JP-8, IPK, and HRJ Camelina have previously been reported [31, 32, 34]; the remaining four fuels were analyzed as part of this work. The results for all nine samples are represented schematically in Fig. Generally speaking, apart from JP-5, all the fuel samples are predominantly composed of linear and branched paraffins and appear to contain significant quantities of monocycloparaffins. Appreciable quantities of aromatics are only observed in the petroleum-derived samples. Additional discussion of the hydrocarbon classification analysis can be found in the accompanying Supplemental Information.

2.2 Experimental Methods

A commercial modulated differential scanning calorimeter (MDSC) was utilized to measure the isobaric specific heat capacity of the nine jet fuel samples. MDSC offers two primary advantages over conventional DSC. First, MDSC allows for the determination of heat capacity from a single experiment rather than the two required with conventional DSC [50-53]. Second, with MDSC, it is possible to separate the total heat flow into a "reversing" (or heat capacity) component and a "nonreversing" (or kinetic) component [50-53]. All measurements in this work utilized a linear heating rate of 3 K·min⁻¹ with a modulation of ± 1 K every 120 s, as well as a continuous purge of 50 mL·min⁻¹ of dry nitrogen. Each sample pan was initially held for 10 min at 183 K before being heated to a maximum temperature of 453 K.

Calibration of temperature, heat flow, and heat capacity are all required for the determination of accurate heat capacities. Details concerning the calibration materials and methods used in this work can be found in the accompanying Supplemental Information. However, it should be noted here that all calibration measurements were performed utilizing the same experimental conditions that were used for the jet fuel samples.

All calibration and jet fuel samples were encapsulated in hermetically sealed aluminum pans, and an empty hermetically sealed pan served as the reference. Details concerning the weighing scheme employed to determine sample masses can be found in the accompanying Supplemental Information. In short, sample masses were determined prior to measurements and then again once measurements were complete to check for mass loss. In this work, just one pan of Jet A was discarded for exhibiting a mass change of > 0.3% [54]. Initially, four pans were prepared for each jet fuel sample; the one exception was Jet A for which a total of 12 pans were prepared. However, concerns that the enthalpy of vaporization could contribute significantly to the apparent heat capacity for low-mass samples, combined with some anomalous measurement results, led to the exclusion of all samples with masses < 7 mg, leaving two or three pans for each fuel (seven for Jet A). The masses of the remaining samples ranged from 7.09 mg to 16.32 mg.

The following procedure was employed for the measurements reported here. Prior to starting sample measurements, the instrument's temperature and heat flow were calibrated as described in the accompanying Supplemental Information. The instrument's performance was verified approximately every 24 h during continuous operation via repeat baseline scans, followed by a single indium measurement. For the jet fuels, the sample pan was placed in the measurement cell and three replicate runs were performed without moving the pan. Measurements for each sample pan were bracketed by a single sapphire calibration run. Ultimately, an average of the 109 separate sapphire calibrations, $\overline{K}_{cp}(T)$ was used to more accurately represent the significant degree of random variability that was observed among the calibration runs. Finally, the instrument's performance and overall procedure were validated via measurements of high-purity hexadecane (Sigma Aldrich, anhydrous, $\geq 99\%$, lot # SHBG2582V).[‡] Hexadecane was chosen because its heat capacity is relatively well known [55] and, as a long-chain hydrocarbon, it is representative of the jet fuel samples. The agreement between hexadecane measurement results and values calculated

[‡]In order to describe materials and experimental procedures adequately, it is occasionally necessary to identify commercial products by manufacturers' names or labels. In no instance does such identification imply endorsement by the National Institute of Standards and Technology, nor does it imply that the particular product or equipment is necessarily the best available for the purpose.

using an equation of state [55] was within approximately 3%; this knowledge was also incorporated into the subsequent uncertainty analysis.

3. Results and Discussion

Averaged isobaric specific heat capacity measurement results (\bar{c}_p) for Jet A, Jet A-1, JP-8, JP-5, S-8, S-5, IPK, HRJ Camelina, and HRJ Tallow are reported in Tables S10–S18 of the Supplemental Information, respectively. It should be noted that only liquid phase data derived from the stable portion of the heat flow curves are presented in Tables S10–S18. Furthermore, the data have been reduced to a point every 1 K to make the amount of tabulated data more manageable.

As was previously discussed, for each fuel, two to three samples were each measured three times for a total of six to nine measurement runs per fuel. For a given fuel, first, replicate measurement results for each pan/mass were averaged (\bar{c}_p), and then those mass averages were averaged together to produce a single overall average (\bar{c}_p); these overall averages are reported in Tables S10–S18. Although three replicate measurements were made for each sample pan, only the second and third replicates have been included in the final data analysis. Most pans measured showed systematically higher values for the first replicate relative to the other two replicates. The lack of observed mass loss for these pans seemed to rule out the loss of very volatile components upon initial heating as an explanation. Efforts were made to verify this conclusion via additional composition measurements, but it was not possible to extract sufficient sample from the sealed pans for testing. However, it should be noted that this phenomenon was also observed with the pure hexadecane samples for which loss of volatile components should not be an issue. Having eliminated compositional changes as an explanation, additional attempts were made to determine if thermal history effects could explain the observed behavior. Even though the thermal history test results were not conclusive, it was decided that the initial replicate measurement would be excluded from the analysis for all sample pans, thus ensuring all pans were treated identically.

The associated absolute expanded uncertainty estimates $(U(\overline{c}_p))$ are also included in Tables S10–S18. These are calculated using the expression

$$U(\bar{\bar{c}}_p) = t_{95} \left(df_{\bar{\bar{c}}_p} \right) \cdot u(\bar{\bar{c}}_p) \tag{1}$$

where the coverage factor, $t_{95} \left(df_{\bar{c}_p} \right)$, is determined from the *t*-distribution for $df_{\bar{c}_p}$ degrees of freedom and a 95% confidence level, and $u(\bar{c}_p)$ is the combined standard uncertainty for the overall average heat capacity [56]. The associated coverage factors have been included in the experimental data tables for clarity. Overall, expanded absolute uncertainties range between 0.025 J·g⁻¹·K⁻¹ and 0.082 J·g⁻¹·K⁻¹, corresponding to relative uncertainties of approximately 1.4% to 2.8%. Additional details regarding the uncertainty analysis can be found in the accompanying Supplemental Information.

The averaged isobaric specific heat capacities shown in Tables S10–S18 are also plotted as a function of temperature in Fig. 2. The plotted data in Fig. 2 have been further limited to a point every 5 K for visual clarity. Generally speaking, the bio-derived fuels exhibit the highest heat capacities, the petroleum-based fuels exhibit the lowest heat capacities, and the synthetic FT fuels fall somewhere in between. Specifically, HRJ Tallow exhibits the highest heat capacities, ranging from 2.015 J·g⁻¹·K⁻¹ at 233 K to 2.869 J·g⁻¹·K⁻¹ at 442 K; the heat capacities for HRJ Camelina are nearly identical, ranging from 2.003 J·g⁻¹·K⁻¹ at 233 K to 2.871 J·g⁻¹·K⁻¹ at 442 K. The relative difference between these two fuels is 0.6% at 233 K and 0.1% at 442 K, significantly less than the estimated experimental uncertainties. At the opposite extreme, petroleum-derived Jet A-1 exhibits heat capacities ranging from 1.721 J·g⁻¹·K⁻¹ at 243 K to 2.501 J·g⁻¹·K⁻¹ at 442 K; the relative

difference in these values from those observed for HRJ Tallow is 18.4% at 243 K and 14.7% at 442 K. Despite all three fuels having very similar fuel specifications [13, 39], both Jet A and JP-8 exhibit higher heat capacities than Jet A-1; JP-8 exhibits the highest heat capacities of the three fuels, ranging from 1.840 J·g⁻¹·K⁻¹ at 243 K to 2.644 J·g⁻¹·K⁻¹ at 442 K, while the heat capacities for Jet A range from 1.802 J·g⁻¹·K⁻¹ at 248 K to 2.580 J·g⁻¹·K⁻¹ at 442 K. The relative differences between JP-8 and Jet A range from 2.8% to 2.5%, which easily fall within the combined estimated uncertainties for these two fuels. Similarly, Jet A has heat capacities that are 4.0% to 3.2% higher than Jet A-1, which still fall within combined estimated uncertainties. In contrast, JP-8 has heat capacities that are 6.9% to 5.7% higher than Jet A-1; these differences exceed combined estimated uncertainties for all but the warmest temperatures (at approximately \geq 430 K). The final petroleum-derived fuel, JP-5, exhibits heat capacities that fall between those of Jet A and Jet A-1, ranging from 1.754 J·g⁻¹·K⁻¹ at 243 K to 2.519 J·g⁻¹·K⁻¹ at 442 K. Interestingly, both S-8 and S-5 exhibit heat capacities that are somewhat higher than the two petroleum-derived fuels they were intended to replace (JP-8 and JP-5, respectively). The heat capacities for S-8 range from 1.964 J·g⁻ 1 ·K⁻¹ at 243 K to 2.751 J·g⁻¹·K⁻¹ at 442 K, which are 6.7% to 4.0% higher than what was observed for JP-8, but it should be noted that such differences fall within combined estimated uncertainties at temperatures of approximately \ge 340 K. For S-5, the observed heat capacities range from 2.020 J·g⁻¹·K⁻¹ at 243 K to 2.819 J·g⁻¹·K⁻¹ at 442 K, corresponding to differences of 15.2% to 11.9% relative to JP-5, which far exceed combined estimated uncertainties. The final synthetic FT fuel, IPK, exhibits heat capacities that are closer to those observed for the petroleum-derived fuels, particularly JP-8, with values ranging from 1.766 J·g⁻¹·K⁻¹ at 223 K to 2.672 J·g⁻¹·K⁻¹ at 442 K. However, it should be noted that the differences between IPK and S-8, which range from 7.3% to 2.9%, do fall within the combined estimated uncertainties for these two fuels at temperatures of approximately \geq 330 K.

Heat capacity is a fundamental extensive property that describes a molecule's or, in our case, a fluid's response to the addition of energy in the form of heat [57]. In the most general terms, when energy is added to a system of complex molecules, there is an increase, not only in the translational motion of the molecules, but also in their rotational, vibrational, and bending motions. Ultimately, the amount of energy required to raise the temperature of a particular amount of a given substance depends upon the molecular structure, as well as the intramolecular and intermolecular interactions. Thus, when considering an unbranched paraffin and its branched counterpart, such as *n*-octane and isooctane, branching effectively lowers the number of possible rotational and vibrational degrees of freedom, which means less energy is required to raise the kinetic energy (i.e., temperature) since more of the energy goes directly to increasing translational motions; this results in a lower heat capacity for isooctane relative to *n*-octane [57]. Alternatively, since the van der Waals forces that primarily determine intermolecular interactions between nonpolar compounds generally increase with increased surface area, the decreased surface area of more compact branched paraffins relative to their unbranched counterparts, results in weaker intermolecular interactions. Thus, less energy is required to overcome these interactions leading to lower heat capacities. Similar arguments can be made for cyclic and aromatic compounds in terms of decreasing rotational degrees of freedom, and thus decreasing heat capacity, moving from unbranched to branched to cyclic to aromatic (e.g., *n*-hexane > 3-methylpentane > cyclohexane > benzene) [57].

While the above considerations can help elucidate how composition contributes to observed heat capacities, they do not necessarily facilitate simple conclusions when dealing with complex mixtures such as fuels. For example, based on the hydrocarbon classification analyses illustrated in Fig. 1, one would expect the two bio-derived and three synthetic fuels to all have similar heat capacities and for their heat capacities to be greater than the four conventional petroleum-derived fuels given the higher linear and branched paraffin content and lower cyclic and aromatic content of the alternative fuels. Fig. 2 demonstrates that this is generally true, although the similarity of IPK to JP-8 is a little surprising given the stark differences in their paraffinic content. Additional apparent inconsistencies start to emerge when we look a little more closely at the chemical composition. For example, the GC-MS results presented in Tables S1–S9 indicate that the bioderived fuels contain more branched paraffins than the synthetic fuels which would theoretically result in lower heat capacities, but this is not the case. Additionally, among the conventional fuels, if the hydrocarbon classification for JP-5 is accurate (Fig. 1), one would expect JP-5 to have the lowest heat capacities given its significantly higher cyclic composition, but, in fact, it is JP-8 that has the lowest heat capacities. This does call into question the validity of the JP-5 classification results, particularly with respect to its relatively high MCP content. However, as was previously discussed, artificially high quantities of monocycloparaffins are unsurprising given that some mass spectral fragments that are supposedly indicative of only MCP are, in actuality, also produced from other paraffinic species [58].

There are limited data available in the literature to which we can compare our heat capacity measurement results. The *Handbook of Aviation Fuel Properties* [11] contains isobaric heat capacity data for Jet A, Jet A-1, JP-8, and JP-5, but it should be noted that the first three fuels are treated as identical. The bulk of reported data were derived from a correlation published by Maxwell [59], which combines averaged fuel specific gravity and distillation data, rather than from experimental heat capacity data. Since the data are only presented graphically, we first had to digitize the graphs and then fit the resulting data points to a straight line to facilitate the calculation of heat capacity values at experimental temperatures for comparison. Additional isobaric heat capacity data for Jet A, Jet A-1, JP-8, and JP-5 are reported by Hadaller and Johnson [60]; they present the results of MDSC measurements for 57 jet fuel samples sourced from 18 countries as

part of the World Fuel Sampling Program. A slope and intercept are reported for each measured fuel sample to facilitate the calculation of isobaric heat capacity as a function of temperature; for the comparisons presented in this work, we compiled the individual fuel sample results and calculated an average slope and intercept for each of the four fuels. Additional MDSC measurement results for Jet A and IPK are reported by Bessee et al. [61]; the reported slopes and intercepts were used to calculate isobaric heat capacities at our experimental temperatures for the comparisons presented here. A final set of MDSC measurement results for Jet A-1 are reported by Zanier and Jäckle [62]; the tabulated data were fit to a straight line to facilitate the calculation of heat capacity values at experimental temperatures for comparison. It should be noted that none of the literature data have been extrapolated beyond their reported temperature ranges. Finally, in addition to the literature data discussed above, our measurement results for Jet A and S-8 can be compared to the predictions of surrogate mixture models. The models [27, 30] were developed at NIST for use with the Reference Fluid Thermodynamic and Transport Properties (REFPROP) program [55].

The data comparison results, plotted as percent deviation as a function of temperature, are summarized in Fig. 3 for Jet A, Jet A-1, JP-8, JP-5, S-8, and IPK; no comparison data could be found for the remaining three fuels (S-5, HRJ Camelina, and HRJ Tallow). For each comparison data source, the same markers have been used throughout to facilitate comparisons between fuels. Additionally, dashed lines have been included to represent the maximum estimated experimental uncertainty limits for each fuel.

The first thing that is readily apparent when looking at Fig. 3 is that there is a significant amount of variability observed among the comparison results. For both Jet A and S-8, very good agreement is observed between experimental measurements and their respective models [27, 30]. Specifically, the absolute average deviation (AAD) for Jet A (Fig. 3a) is 0.4% with an overall

range of -1.3% to 0.5%; for S-8 (Fig. 3e) the AAD is 0.9%, and the deviations range from -1.0%to 1.9%. Similarly, relatively good agreement is observed for the results of Bessee et al. [61] for Jet A (Fig. 3a), with deviations ranging from -3.0% to -0.4% and an AAD of 1.4%, but the agreement is slightly worse for IPK (Fig. 3f), with deviations ranging from 0.5% to 3.9%, and an AAD of 3.0%. The situation generally improves with the values from the Handbook of Aviation Fuel Properties [60], which agree with our results, within experimental uncertainties, for Jet A (Fig. 3a), JP-8 (Fig. 3c), and JP-5 (Fig. 3d), with AADs of 1.1%, 1.3%, 2.4%, respectively. The overall deviations for these fuels range from 0.7% to 1.3% for Jet A, from -2.1% to -1.1% for JP-8, and from 1.9% to 2.7% for JP-5. However, values from the Handbook of Aviation Fuel *Properties* [60] for Jet A-1 (Fig. 3b) are 4.0% to 5.3% higher than our experimental results, with an AAD of 5.0%, far exceeding estimated uncertainties. For Jet A-1 (Fig. 3b), even larger deviations are observed with the data of Zanier and Jäckle [62], ranging from 6.8% to 9.7%, with an AAD of 8.8%. Finally, Fig. 3 clearly shows that, in every case, the results from the World Fuel Sampling Program reported by Hadaller and Johnson [60] are significantly lower than both the experimental results reported herein, and the other available literature data. Specifically, for Jet A (Fig. 3a), deviations range from -19.5% to -16.4%, with an AAD of 16.9%. For Jet A-1 (Fig. 3b), the deviations range from -13.3% to -9.7%, with an AAD of 10.4%. The deviations for JP-8 (Fig. 3c) range from -19.6% to -15.8%, with an AAD of 16.5%; while deviations for JP-5 (Fig. 3d) range from -17.7% to -15.0%, with an AAD of 15.5%. Finally, for IPK (Fig. 3f), deviations range from -22.0% to -18.8%, with an AAD of 19.5%. It should be noted that, unlike the other four fuels for which the reported data represent an average of multiple samples that were collected and measured as part of the World Fuel Sampling Program, the reported data for IPK are from a single sample [60].

As was previously discussed, fuel standards are primarily performance specifications rather than strict compositional specifications since differences in crude sources and manufacturing processes are expected to introduce a significant degree of variability among resulting fuel products [13]; past research has demonstrated that the variability extends to certain fuel properties as well [34, 36, 63]. Consequently, it would be reasonable to assume that at least some of the differences in heat capacities observed in Fig. 3 can be attributed to compositional variability among fuel batches. Unfortunately, specific batch information was not provided in any of the source references. In the case of the World Fuel Sampling Program data reported by Hadaller and Johnson [60], significant differences in measurement protocols seem the most likely explanation for the large observed deviations. As was the case with the results reported in this work, the data reported by Bessee et al. [61], Zanier and Jäckle [62], and Hadaller and Johnson [60] were all derived from MDSC measurements. Differences in key experimental parameters such as purge gas, modulation conditions, and underlying heating rate will inevitably result in a reasonable degree of variability among measurement results. In the case of the World Fuel Sampling Program data, the underlying heating rate employed was drastically different from any of the other data sets. Specifically, Hadaller and Johnson [60] report that a heating rate of 20 K min⁻¹ was used; this is significantly higher than the 3 K·min⁻¹ employed by Bessee et al. [61], the 2 K·min⁻¹ employed by Zanier and Jäckle [62], and the 3 K min⁻¹ employed in this work. This is significant because MDSC assumes that the temperature as measured at the cell platform is representative of the encapsulated sample temperature and that temperature gradients within the sample are minimal. The higher the heating rate, the greater the chance that these assumptions no longer hold; assuming heat capacity increases with increasing temperature, this would manifest as negatively biased results. In fact, Hadaller and Johnson [60] report additional data from measurements performed several months after the initial measurement phase was complete that appear to support this hypothesis.

Specifically, there were six new Jet A-1 samples and a single repeat IPK sample that were measured during this second phase following an altered measurement protocol, the largest difference being the use of a much slower underlying heating rate of 5 K min⁻¹ [60]. These data are shown in Fig. 3b and Fig. 3f for comparison. For the six new Jet A-1 samples (Fig. 3b), the averaged measurement results are approximately 5.4% to 6.0% higher than the earlier averaged results for 25 samples measured at 20 K·min⁻¹ [60]. Relative to the Jet A-1 data from this work, the six new World Fuel Sampling Program samples [60] show deviations of -8.1% to -4.6%, with an AAD of 5.3%. The impact of a slower heating rate is even more apparent for IPK where the same single sample was measured using the two different measurement protocols (Fig. 3f). Here, the later measurements produced results that are approximately 15.0% to 18.2% higher than the initial data [60], and that deviate by approximately -7.8% to -5.8%, with an AAD of 6.3%, relative to the IPK results reported in this work. Although the deviations still exceed estimated experimental uncertainties in both cases, the data using the slower heating rate represent a significant improvement over initial results, bringing the World Fuel Sampling Program data closer in line with other available data.

Finally, to facilitate their use, the experimental data reported herein have been correlated as a function of temperature using the expression

$$\bar{c}_p = \alpha_0 + (\alpha_1 \cdot T) + (\alpha_2 \cdot T^2) + (\alpha_3 \cdot T^3).$$
(2)

Table 1 contains the resulting coefficients and associated standard uncertainties for all nine fuel samples. Also shown in Table 1 are the observed AADs for calculated isobaric heat capacities relative to experimental values. Additionally, the relative deviations between calculated and experimental values are plotted as a function of temperature in Fig. 4 for all nine fuels. In all cases, these deviations are approximately an order of magnitude smaller than estimated experimental uncertainties. The overall best fit is observed for HRJ Camelina with deviations ranging from

approximately -0.38% to approximately 0.16%; the overall worst fit is observed for Jet A-1 with deviations ranging from approximately -0.28% to approximately 0.25%.

4. Conclusions

In this work, isobaric heat capacity measurements for nine aviation turbine fuel samples have been presented. The nine samples represent a variety of fuel types including conventional, synthetic, and renewable fuels. All measurements were made using MDSC over the combined temperature range of (223 to 442) K. Significant variability was observed among the nine samples; the overall spread in isobaric heat capacity ranged from 18.4% at 243 K to 14.7% at 442 K. Generally speaking, the bio-derived fuels exhibited the highest heat capacities, the petroleumbased fuels exhibited the lowest heat capacities, and the synthetic FT fuels fell somewhere in between. Additionally, both S-8 and S-5 exhibited heat capacities that were somewhat higher than the two petroleum-derived fuels they were intended to replace (JP-8 and JP-5, respectively); while the final synthetic FT fuel, IPK, exhibited heat capacities that were closer to those observed for the petroleum-derived fuels, particularly JP-8. In addition to the fuel-to-fuel comparisons, measurement results for the nine fuels were compared with available literature data and existing surrogate mixture models. In most instances, the calculated deviations were within estimated experimental uncertainties. The most glaring exception was for the data from the World Fuel Sampling Program [60], which, in all cases, were significantly lower than both the experimental results reported in this work and other available data. Evidence suggests that a significantly faster heating rate is the cause for the large observed differences. As was previously mentioned, an understanding of the basic thermodynamic properties of a fuel is critical in the search for sustainable aviation fuel sources. It is our hope that the data reported here, and within the related paper of Fortin and Bruno [23], will aid the community in its search.

Acknowledgments

We acknowledge the Propulsion Directorate of the Air Force Research Laboratory at Wright-Patterson Air Force Base for providing the fuel samples measured in this work. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Supplemental Information

The online version contains supplementary material available at https://doi. org/10.1007/s10765-022-03100-2.

Declarations

Competing Interest

The authors have no relevant financial or non-financial interests to disclose.

Author Contributions

Tara J. Fortin: Conceptualization, Methodology, Formal Analysis and Investigation, Writing – original draft preparation. Thomas J. Bruno: Supervision, Writing – review and editing. Tara M. Lovestead: Formal Analysis and Investigation, Writing – review and editing.

Data Availability

Experimental data from this study are included in Tables S10–S18 of the Supplemental Information file. The data are also available in digital format online at https://doi.org/10.18434/mds2-2691.

References

[1] *Annual Report of the Council* (International Civil Aviation Organization, Montréal, Canada, 2018)

[2] IATA Annual Review 2018 (International Air Transport Association, Montréal, Canada, 2018)

[3] 2019 Environmental Report: Aviation and Environment (International Civil Aviation Organization, Montréal, Canada, 2019)

[4] A Global Approach to Reducing Aviation Emissions (International Air Transport Association, Montréal, Canada, 2009)

[5] *Group on International Aviation and Climate Change (GIACC) Report* (International Civil Aviation Organization, Montréal, Canada, 2009)

[6] Aviation Environmental and Energy Policy Statment (Federal Aviation Administration, Washington, DC, USA, 2012)

[7] D.L. Daggett, R.C. Hendricks, R. Walther, E. Corporan, *Alternative Fuels for Use in Commercial Aircraft*, NASA/TM-2008-214833 (NASA Center for Aerospace Information, Hanover, MD, USA, 2008)

[8] K. Lewis, S. Mitra, S. Xu, L. Tripp, M. Lau, A. Epstein, G. Fleming, C. Roof, *Alternative Jet Fuel Scenario Analysis Report*, DOT-VNTSC-FAA-12-01 (John A. Volpe National Transportation Systems Center, Cambridge, MA, USA, 2012)

[9] *IATA 2015 Report on Alternative Fuels* (International Air Transport Association, Montréal, Canada, 2015)

[10] Sustainable Aviation Fuels Guide (International Civial Aviation Organization, Montréal, Canada, 2017)

[11] *Handbook of Aviation Fuel Properties*, CRC Report 635 (Coordinating Research Council, Inc., Alpharetta, GA, USA, 2004)

[12] World Jet Fuel Specifications with Avgas Supplement (ExxonMobil Aviation, Brussels, Belgium, 2008)

[13] *Standard Specification for Aviation Turbine Fuels*, ASTM D1655-19a (ASTM International, West Conshohocken, PA, USA, 2019)

[14] N. Winchester, D. McConnachie, C. Wollersheim, I. Waitz, *Market Cost of Renewable Jet Fuel Adoption in the United States: A PARTNER Project 31 Report*, PARTNER-COE-2013-001

(The Partnership for Air Transportation Noise and Emissions Reduction (PARTNER), Cambridge, MA, USA, 2013)

[15] Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons, ASTM D7566-21 (ASTM International, West Conshohocken, PA, USA, 2021)

[16] *IATA 2013 Report on Alternative Fuels* (International Air Transport Association, Montréal, Canada, 2013)

[17] Heathrow Reduces Emissions with SAF, <u>https://www.heathrow.com/latest-news/sustainable-aviation-fuel-to-partly-power-heathrow-jets</u> (accessed August 31, 2021)

[18] A. Milbrandt, C. Kinchin, R. McCormick, *The Feasibility of Producing and Using Biomass-Based Diesel and Jet Fuel in the United States*, NREL/TP-6A20-58015 (National Renewable Energy Lab, Golden, CO, USA, 2013)

[19] E. Corporan, R.Q. Casselberry, M.J. DeWitt, Gas-Phase Pyrolysis Characteristics of Hydrocarbon Fuels and Their Potential Impacts on Combustion Operational Performance. Energy Fuels **34**, 14843-14852 (2020)

[20] R. Alsulami, B. Windom, Liquid Jet Fuel Property Impacts on Combustion Performance. J. Propuls. Power **37**, 276-282 (2021)

[21] J.L. Burton, J.A. Martin, G.M. Fioroni, T.L. Alleman, C.K. Hays, M.A. Ratcliff, M.R. Thorson, A.J. Schmidt, R.T. Hallen, T.R. Hart, J.M. Billing, S. Fox, D.J. Gaspar, J. Zhu, C. Kima, L.D. Pfefferle, C.S. McEnally, R.L. McCormick, *Fuel Property Effects of a Broad Range of Potential Biofuels on Mixing Control Compression Ignition Engine Performance and Emissions*, SAE Technical Paper 2021-01-0505 (Society of Automotive Engineers (SAE), Warrendale, PA, USA, 2021)

[22] J.-D. Woodroffe, D.V. Lupton, M.D. Garrison, E.M. Nagel, M.J. Siirila, B.G. Harvey, Synthesis and Fuel Properties of High-Energy Density Cyclopropanated Monoterpenes. Fuel Process. Technol. **222**, 106952 (2021)

[23] T.J. Fortin, T.J. Bruno, Heat Capacity Measurements of Conventional Aviation Fuels. Fuel Process. Technol. **235**, 107341 (2022)

[24] T.J. Bruno, B.L. Smith, Improvements in the Measurement of Distillation Curves. 2. Application to Aerospace/Aviation Fuels RP-1 and S-8. Ind. Eng. Chem. Res. 45, 4381-4388 (2006)

[25] B.L. Smith, T.J. Bruno, Improvements in the Measurement of Distillation Curves. 4. Application to the Aviation Turbine Fuel Jet-A. Ind. Eng. Chem. Res. **46**, 310-320 (2007)

[26] T.J. Bruno, A. Laesecke, S.L. Outcalt, H.D. Seelig, B.L. Smith, *Properties of a 50/50 Mixture of Jet-A* + *S-8*, NISTIR 6647 (National Institute of Standards and Technology, Boulder, CO, USA, 2007)

[27] M.L. Huber, B.L. Smith, L.S. Ott, T.J. Bruno, Surrogate Mixture Model for the Thermophysical Properties of Synthetic Aviation Fuel S-8: Explicit Application of the Advanced Distillation Curve. Energy Fuels **22**, 1104-1114 (2008)

[28] J.A. Widegren, T.J. Bruno, Thermal Decomposition Kinetics of the Aviation Turbine Fuel Jet A. Ind. Eng. Chem. Res. 47, 4342-4348 (2008)

[29] S.L. Outcalt, A. Laesecke, M.B. Freund, Density and Speed of Sound Measurements of Jet A and S-8 Aviation Turbine Fuels. Energy Fuels **23**, 1626-1633 (2009)

[30] M.L. Huber, E.W. Lemmon, T.J. Bruno, Surrogate Mixture Models for the Thermophysical Properties of Aviation Fuel Jet-A. Energy Fuels **24**, 3565-3571 (2010)

[31] T.J. Bruno, E. Baibourine, T.M. Lovestead, Comparison of Synthetic Isoparaffinic Kerosene Turbine Fuels with the Composition-Explicit Distillation Curve Method. Energy Fuels **24**, 3049-3059 (2010)

[32] T.J. Bruno, E. Baibourine, Comparison of Biomass-Derived Turbine Fuels with the Composition-Explicit Distillation Curve Method. Energy Fuels **25**, 1847-1858 (2011)

[33] S.L. Outcalt, T.J. Fortin, Density and Speed of Sound Measurements of Two Synthetic Aviation Turbine Fuels. J. Chem. Eng. Data **56**, 3201-3207 (2011)

[34] J.L. Burger, T.J. Bruno, Application of the Advanced Distillation Curve Method to the Variability of Jet Fuels. Energy Fuels **26**, 3661-3671 (2012)

[35] S.L. Outcalt, T.J. Fortin, Density and Speed of Sound Measurements of Four Bioderived Aviation Fuels. J. Chem. Eng. Data **57**, 2869-2877 (2012)

[36] T.J. Fortin, A. Laesecke, Viscosity Measurements of Aviation Turbine Fuels. Energy Fuels **29**, 5495-5506 (2015)

[37] T.M. Lovestead, J.L. Burger, N. Schneider, T.J. Bruno, Comprehensive Assessment of Composition and Thermochemical Variability by High Resolution GC/QToF-MS and the Advanced Distillation-Curve Method as a Basis of Comparison for Reference Fuel Development. Energy Fuels **30**, 10029-10044 (2016)

[38] L.Q. Maurice, H. Lander, T. Edwards, W.E. Harrison, Advanced Aviation Fuels: A Look Ahead via a Historical Perspective. Fuel **80**, 747-756 (2001)

[39] Detail Specification Turbine Fuel, Aviation, Kerosene Type, JP-8 (NATO F-34), NATO F-35, and JP-8+100 (NATO F-37), MIL-DTL-83133J (Air Force Petroleum Office, Wright-Patterson Air Force Base, OH, USA, 2015)

[40] *Detail Specification Turbine Fuel, Aviation, Grades JP-4 and JP5*, MIL-DTL-5624W (Air Force Petroleum Office, Wright-Patterson Air Force Base, OH, USA, 2016)

[41] F. Fischer, H. Tropsch, The Synthesis of Petroleum at Atmospheric Pressures from Gassification Products of Coal. Brennst.-Chem. 7, 97-104 (1926)

[42] C.A. Moses, *Comparative Evaluation of Semi-Synthetic Jet Fuels: Final Report*, AV-2-04a (Coordinating Research Council, Inc., Alpharetta, GA, USA, 2008)

[43] P.A. Muzzell, R.L. Freerks, J.P. Baltrus, D.D. Link, Composition of Syntroleum S-5 and Conformance to JP-5 Specification. Prepr. Pap. Am. Chem. Soc. Div. Petrol. Chem. **49**, 411-413 (2004)

[44] C. Ciubota-Rosie, J.R. Ruiz, M.J. Ramos, A. Pérez, Biodiesel from *Camelina sativa*: A Comprehensive Characterisation. Fuel **105**, 572-577 (2013)

[45] R.J. Roseberg, R.A. Bentley, *Growth, Seed Yield, and Oil Production of Spring Camelina sativa in Response to Irrigation Rate and Harvest Method, in the Klamath Basin, 2011* (Oregon State University Klamath Basin Research & Extension Center (KBREC), Corvallis, OR, USA, 2011)

[46] D.R. Shonnard, L. Williams, T.N. Kalnes, Camelina-Derived Jet Fuel and Diesel: Sustainable Advanced Biofuels. Environ. Prog. Sustain. Energy **29**, 382-392 (2010)

[47] W.-C. Wang, L. Tao, Bio-Jet Fuel Conversion Technologies. Renew. Sust. Energ. Rev. 53, 801-822 (2016)

[48] Standard Test Method for Hydrocarbon Types in Low Olefinic Gasoline by Mass Spectrometry, ASTM D2789-95(2016) (ASTM International, West Conshohocken, PA, USA, 2016)

[49] B.L. Smith, T.J. Bruno, Improvements in the Measurement of Distillation Curves. 3. Application to Gasoline and Gasoline + Methanol Mixtures. Ind. Eng. Chem. Res. 46, 297-309 (2007)

[50] J. Boerio-Goates, J.E. Callanan, Differential Thermal Methods, in *Physical Methods of Chemistry, Volume VI: Determination of Thermodynamic Properties*, ed. by B.W. Rossiter, R.C. Baetzold (John Wiley & Sons, New York, NY, USA, 1992), pp 621-717

[51] M. Reading, A. Luget, R. Wilson, Modulated Differential Scanning Calorimetry. Thermochim. Acta **238**, 295-307 (1994)

[52] B. Wunderlich, Y. Jin, A. Boller, Mathematical Description of Differential Scanning Calorimetry Based on Periodic Temperature Modulation. Thermochim. Acta **238**, 277-293 (1994)

[53] G.W.H. Höhne, W. Hemminger, H.J. Flammersheim, *Differential Scanning Calorimetry: An Introduction for Practitioners* (Springer-Verlag, Berlin, Germany, 1996)

[54] Standard Test Method for Determining Specific Heat Capacity by Differential Scanning Calorimetry, ASTM E1269-11 (ASTM International, West Conshohocken, PA, USA, 2011)

[55] E.W. Lemmon, I.H. Bell, M.L. Huber, M.O. McLinden, *NIST Standard Reference Database* 23: *Reference Fluid Thermodynamic and Transport Properties (REFPROP)*, 10.0 (National Institute of Standards and Technology, Gaithersburg, MD, USA, 2018)

[56] *Guide to the Expression of Uncertainty in Measurement* (International Organization for Standardization, Geneva, Switzerland, 1995)

[57] R. Naef, Calculation of the Isobaric Heat Capacities of the Liquid and Solid Phase of Organic Compounds at and Around 298.15 K Based on Their "True" Molecular Volume. Molecules **24**, 1626 (2019)

[58] T.J. Bruno, P.D.N. Svoronos, *CRC Handbook of Basic Tables for Chemical Analysis - Data Driven Methods and Interpretation* (CRC Press, Taylor & Francis Group, Boca Raton, FL, USA, 2021)

[59] J.B. Maxwell, *Data Book on Hydrocarbons: Application to Process Engineering* (Van Nostrand Co., Princeton, NJ, USA, 1957)

[60] O.J. Hadaller, J.M. Johnson, *World Fuel Sampling Program*, CRC Report 647 (Coordinating Research Council, Inc., Alpharetta, GA, USA, 2006)

[61] G.B. Bessee, S.A. Hutzler, G.R. Wilson, *Analysis of Synthetic Aviation Fuels: Interim Report*, AFRL-RZ-WP-TR-2011-2084 (Air Force Research Laboratory, Wright-Patterson Air Force Base, OH, USA, 2011)

[62] A. Zanier, H.W. Jäckle, Heat Capacity Measurements of Petroleum Fuels by Modulated DSC. Thermochim. Acta **287**, 203-212 (1996)

[63] T.J. Fortin, Assessment of Variability in the Thermophysical Properties of Rocket Propellant RP-1. Energy Fuels **26**, 4383-4394 (2012)

Fuel	a	$u(\alpha_0)$	α_1	$u(\alpha_1)$	α_2	$u(\alpha_2)$	<i>0</i> (3	$u(\alpha_3)$	AAD ^a
	$/J \cdot g^{-1} \cdot K^{-1}$	$/J \cdot g^{-1} \cdot K^{-1}$	$/J \cdot g^{-1} \cdot K^{-2}$	$/J \cdot g^{-1} \cdot K^{-2}$	$/J \cdot g^{-1} \cdot K^{-3}$	$/J \cdot g^{-1} \cdot K^{-3}$	$/J \cdot g^{-1} \cdot K^{-4}$	$/J \cdot g^{-1} \cdot K^{-4}$	/%
Jet A	1.9729	0.0297	-5.5109E-03	2.6532E-04	2.4311E-05	7.7840E-07	-1.9803E-08	7.5090E-10	0.056
Jet A-1	1.7691	0.0375	-3.8864E-03	3.3816E-04	1.8243E-05	1.0002E-06	-1.2952E-08	9.7177E-10	0.086
JP-8	1.9028	0.0344	-4.4277E-03	3.0977E-04	2.1105E-05	9.1620E-07	-1.6571E-08	8.9021E-10	0.065
JP-5	1.8179	0.0267	-4.2908E-03	2.4028E-04	2.0438E-05	7.1068E-07	-1.6186E-08	6.9052E-10	0.057
S-8	1.9980	0.0337	-3.8220E-03	3.0355E-04	1.8239E-05	8.9780E-07	-1.2981E-08	8.7233E-10	0.057
S-5	2.0561	0.0393	-4.0889E-03	3.5453E-04	1.9766E-05	1.0486E-06	-1.4896E-08	1.0188E-09	0.068
IPK	1.7665	0.0243	-3.5859E-03	2.2783E-04	1.9314E-05	6.9674E-07	-1.4886E-08	6.9708E-10	0.068
HRJ Camelina	2.4806	0.0198	-7.8727E-03	1.8139E-04	3.0642E-05	5.4543E-07	-2.4532E-08	5.3771E-10	0.043
HRJ Tallow	2.2463	0.0307	-5.5908E-03	2.8180E-04	2.3854E-05	8.4734E-07	-1.8147E-08	8.3535E-10	0.068

Table 1 Coefficients (α_i) and Associated Standard Uncertainties ($u(\alpha_i)$) from the Fit of Eq. 2 to Experimental Isobaric Heat Capacity Data for Nine Aviation Fuels

^aThe average absolute deviation (AAD) between experimental data and fit results.

Figure Captions

Fig. 1 Schematic representation of ASTM Method D-2789 [48] hydrocarbon classification analysis results for nine jet fuel samples. Measured percent volume fractions are shown for each of six families: paraffins (P), monocycloparaffins (MCP), dicycloparaffins (DCP), alkylbenzenes (AB), indanes and tetralins (I&T), and naphthalenes (N). Analysis results for Jet A, Jet A-1, JP-8, IPK, and HRJ Camelina have previously been reported [31, 32, 34]; the remaining four fuels were analyzed as part of this work

Fig. 2 Averaged isobaric specific heat capacities for nine jet fuels plotted as a function of temperature. For clarity, data are only plotted every 5 K. Expanded absolute uncertainties for the nine fuels are as follows: $0.025-0.036 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for Jet A (\bigcirc), $0.049-0.071 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for Jet A-1 (\diamondsuit), $0.050-0.075 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for JP-8 (*), $0.048-0.072 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for JP-5 (×), $0.043-0.062 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for S-8 (*), $0.055-0.080 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for S-5 (\square), $0.049-0.076 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for IPK (\bigcirc), $0.055-0.082 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for HRJ Camelina (+), and $0.055-0.082 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ for HRJ Tallow (\triangle) **Fig. 3** Comparisons of available isobaric heat capacity data with measurement results from this work, plotted as percent deviation as a function of temperature. Deviation plots are shown for (a) Jet A, (b) Jet A-1, (c) JP-8, (d) JP-5, (e) S-8, and (f) IPK. Values derived from corresponding surrogate mixture models [27, 30] (*) are included for Jet A and S-8. Literature data from the *Handbook of Aviation Fuel Properties* [11] (\bigcirc), Hadaller and Johnson [60] (\square), Bessee et al. [61] (\triangle), and Zanier and Jäckle [62] (\diamondsuit) are included where available. For both Jet A-1 and IPK, additional data from Hadaller and Johnson [60] (\blacksquare) have also been included; these data are derived from a second round of measurements performed several months after completion of the

initial phase. The dashed lines represent the maximum estimated experimental uncertainty limits for each fuel

Fig. 4 Relative deviations for the correlation of experimental isobaric heat capacity data with Eq.

2. Symbols are as follows: O, Jet A; ♦, Jet A-1; *, JP-8; ×, JP-5; X, S-8; □, S-5; △, IPK; +,

HRJ Camelina; and \triangle , HRJ Tallow



Fig. 1 Schematic representation of ASTM Method D-2789 [48] hydrocarbon classification analysis results for nine jet fuel samples. Measured percent volume fractions are shown for each of six families: paraffins (P), monocycloparaffins (MCP), dicycloparaffins (DCP), alkylbenzenes (AB), indanes and tetralins (I&T), and naphthalenes (N). Analysis results for Jet A, Jet A-1, JP-8, IPK, and HRJ Camelina have previously been reported [31, 32, 34]; the remaining four fuels were analyzed as part of this work



Fig. 2 Averaged isobaric specific heat capacities for nine jet fuels plotted as a function of temperature. For clarity, data are only plotted every 5 K. Expanded absolute uncertainties for the nine fuels are as follows: $0.025-0.036 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for Jet A (O), $0.049-0.071 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for Jet A-1 (\diamond), $0.050-0.075 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for JP-8 (*), $0.048-0.072 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for JP-5 (\times), $0.043-0.062 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for S-8 (X), $0.055-0.080 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for S-5 (\Box), $0.049-0.076 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for IPK (\diamond), $0.055-0.082 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for HRJ Camelina (+), and $0.055-0.082 \text{ J}\cdot\text{g}^{-1}\cdot\text{K}^{-1}$ for HRJ Tallow (Δ)



Fig. 3 Comparisons of available isobaric heat capacity data with measurement results from this work, plotted as percent deviation as a function of temperature. Deviation plots are shown for (a) Jet A, (b) Jet A-1, (c) JP-8, (d) JP-5, (e) S-8, and (f) IPK. Values derived from corresponding surrogate mixture models [27, 30] (*) are included for Jet A and S-8. Literature data from the *Handbook of Aviation Fuel Properties* [11] (O), Hadaller and Johnson [60] (\square), Bessee et al. [61] (\triangle), and Zanier and Jäckle [62] (\diamondsuit) are included where available. For both Jet A-1 and IPK, additional data from Hadaller and Johnson [60] (\square) have also been included; these data are derived from a second round of measurements performed several months after completion of the initial phase. The dashed lines represent the maximum estimated experimental uncertainty limits for each fuel



Fig. 4 Relative deviations for the correlation of experimental isobaric heat capacity data with Eq. 2. Symbols are as follows: O, Jet A; \diamondsuit , Jet A-1; *, JP-8; \times , JP-5; Ξ , S-8; \Box , S-5; \circlearrowright , IPK; +, HRJ Camelina; and \triangle , HRJ Tallow