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Extent and Impacts of Hydrocarbon Fuel Compositional Variability for Aerospace Propulsion Systems

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Kerosene fuels possess physical and chemical properties which make them attractive for aerospace propulsion applications from operational and performance standpoints. However, variation in fuel properties and performance owing to differences in chemical makeup can be significant as fuel composition and operating environments fall outside the realm of current experience. Both circumstances are increasingly frequent, given the incorporation of new fuels in existing systems and a desire to increase vehicle performance. The Air Force Research Laboratory (AFRL) is engaged in deriving relationships between fuel composition, properties, and performance in realistic operating conditions. Ideally, these models will be implemented in the optimization of fuel composition to meet requirements for future systems. Moreover, current engine development activities prompt an assessment of as-supplied rocket kerosene, the set of requirements used for its specification, and the potential impacts of compositional variations on engine operability and performance. To address these needs, several lab scale RP-1 formulations were obtained which met specification requirements but were blended from chemically unique feedstocks, thereby representing the expected compositional variation for currently produced fuel. Chemical composition was characterized in terms of hydrocarbon types and was compared between the various blends. Several property measurements provided insight to compositional influence on fuel behavior; reported in this paper are composition explicit distillation curve, density, viscosity, heat of combustion, and hydrogen content. While chemical variability for RP-1 was not as extensive as that of jet fuel, the sensitivity of several properties to feedstock selection was demonstrated, even for fuels which met specification requirements.

I. Introduction

HYDROCARBON fuels are widely used in aerospace propulsion platforms due to attractive physical and chemical characteristics. Early reciprocating engine aircraft were benefactors of advancing fuel production technology, while the introduction of gas turbine engines to aviation prompted the development of a rigorous jet fuel specification for a growing fleet.¹ As engine performance and thereby aircraft operational capabilities advanced, jet fuel production and specification progressed to meet flight requirements while maintaining a balance with availability and cost.² Specialty fuels and additives have enabled safe performance in circumstances requiring unique operation, such as high altitude and long duration flights.³ Experience gained in fuel development efforts for

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subsonic applications led to consideration of liquid hydrocarbon fuels for high speed flight. Density and handling/storage benefits are among the criteria used in selecting liquid hydrocarbons for certain flight regimes of high Mach number ($M > 5$) applications.^{4, 5} Trade analyses for the purpose of propellant selection have also been conducted for liquid rocket propulsion systems. In particular, booster stages of expendable or reusable launch vehicles often favor hydrocarbon fuels over hydrogen due to their relatively high density and the cost associated with storing and handling cryogenic hydrogen.^{6, 7} Experience gained during previous kerosene engine development efforts is also an important consideration for future launch systems.⁸ (In the context of this paper, the term kerosene is used conventionally to describe the middle distillate range of hydrocarbons found in practical aerospace fuels, regardless of the original source.) Therefore, for subsonic and high speed flight as well as space access applications, kerosene fuels have enabled performance and operational requirements; this has occurred largely through identifying and specifying fuel formulations which meet given engine and fuel system needs.

Variation in fuel properties and performance owing to differences in chemical makeup can be significant as operating environments and fuel composition fall outside the realm of current experience. Both circumstances are increasingly frequent, given the incorporation of new fuels in existing systems and a desire to increase vehicle performance. The Air Force Research Laboratory (AFRL) is currently involved in deriving relationships between fuel composition, physical and chemical properties, and performance in realistic operating conditions. Ideally, these models will be incorporated in the optimization of fuel composition to meet requirements for future systems in the areas of alternative fuels certification, hypersonic vehicles, and liquid rocket propulsion systems. In this paper, we review current specification requirements; identify needs for improved characterization of fuel composition; and compare variability in chemical composition and properties. We accomplish this by assessing the compositional variability of a set of chemically unique rocket grade kerosene batches and comparing with survey results for conventional (petroleum-derived) jet fuel. As part of a longer-term effort in composition-based fuel property modeling, we present several thermophysical property data indicating the impacts of fuel compositional variation.

II. Current Specification Approach and Emerging Compositional Needs

Aerospace kerosene fuels are specified primarily by physical property and compositional limits based on hardware-specific performance. Table 1 compares some detail specification (MIL-spec) requirements which govern product conformance (whether or not a fuel “meets spec”) for several aerospace fuels. Fuel composition is dependent on source material and production methods, while properties are dependent on chemical composition and to some extent analysis method. Fuel performance and suitability for a given propulsion system are not specified *per se*, but are implied through quantitative property and composition limits. For example, a relatively narrow density range for RP-1/RP-2 compared with aviation fuels reflects the sensitivity of rocket engine and launch vehicle performance to density fluctuations. Likewise, relatively low sulfur levels are permitted in rocket kerosene in an attempt to minimize surface fouling due to corrosive copper-sulfur reactions leading to deposit buildup in copper-based regenerative cooling passages.⁹ Vapor pressure requirements (not shown) and distillation temperature limits for JP-7 permit safe fuel system operation under high heat loads accompanying supersonic flight, while shipboard storage safety concerns impose a higher flash point for JP-5 than for its ground-stored counterpart, JP-8.³ Note that compositional requirements exist largely through limitations on certain constituents (e.g., mercaptan sulfur), but fuel composition in terms of hydrocarbon classes such as straight chain (*n*-), branched (*iso*-), and cyclic paraffins is not specified. In this sense, final product composition is an artifact of “upstream” influences but is somewhat unconstrained provided that specification requirements are met. This feature of property-based specification results in fuels which may vary in chemical makeup from one production lot to another, even within the allowable specification.

Commonality among current aerospace propulsion technologies requires improved characterization of the extent and impacts of compositional variability for three primary reasons: the certification and use of fuels with significantly different chemical makeup in legacy aircraft and engine systems; the opportunity to exploit fuel composition in order to meet unprecedented performance and lifecycle requirements; and the increasing role of computational modeling in the design of aerospace combustion devices.

Fuel properties play an important role in Air Force and commercial efforts to certify alternative (non-petroleum) aviation fuels for use in existing aircraft engines. The current goal is to qualify “drop-in” replacements for conventional fuels such as Jet A and JP-8, which requires physical properties and behavior to fall within the experience base of current fuels.¹⁰ Given the variety of alternative fuel sources and processing routes, chemical composition of emerging alternative jet fuel blendstock candidates can vary widely. Extensive physical property measurement efforts for each formulation or blend are impractical. Instead, predictive models are sought which are capable of correlating fuel composition with specified properties and indicators of performance. The development of

Table 1. Selected Specification Requirements for Current Aerospace Fuels

	ASTM Method	JP-5 MIL-DTL-5624U	JP-7 MIL-DTL-38219D	JP-8 MIL-DTL-83133G	RP-1 ^a MIL-DTL-25576E	RP-2 ^a MIL-DTL-25576E
Requirement, Units						
Distillation, °C						
IBP	D86 ^b	report	>182	report	report	report
10% recovered		<205	>196	<205	(185-210)	(185-210)
20% recovered		report	>206	report		
50% recovered		report	report	report	report	report
90% recovered		report	<260	report	report	report
End point		<300	<288	<300	(<274)	(<274)
Density/15°C, kg/L	D1298/ D4052 ^c	0.788-0.845	0.779-0.806	0.775-0.840	0.799-0.815	0.799-0.815
Viscosity/-20°C, mm ² /s	D445	<8.5	<8.0	<8.0	<16.5 ^d	<16.5 ^d
Flash Point, °C	D93	>60	>60	>38	(>60)	(>60)
Freezing Point, °C	D2386	<-46 ^e	<-43.3	<-47 ^f	(<-51)	(<-51)
Net Heat of Combustion, MJ/kg	varies ^g	>42.6	>43.5	>42.8	(>43.0)	(>43.0)
Hydrogen, mass %	varies ^h	>13.4	>14.4	>13.4	>13.8	>13.8
Aromatics, vol %	D1319	<25.0	<5	<25.0	<5	<5
Olefins, vol %	D1319				<2.0	<1.0
Total sulfur, mass%	varies ⁱ	<0.3	<0.1	<0.3	<0.003	<0.00001
Mercaptan sulfur, mass%	D3227	<0.002 ^j	<0.001 ^j	<0.002 ^j	<0.0003	
Thermal Stability: ΔP change, mmHg	D3241/ JFTOT	<25 (260C, 150 min.)	<25 (355C, 300 min.)	<25 (260C, 150 min.)		report (355C, 300 min.)

Notes:

^a Parentheses denote unit conversion from detail specification.

^b JP-5 and JP-8 also allow D2887.

^c Either method may be used. (For dispute, JP-5, JP-7, JP-8 use D4052; RP-1, RP-2 use D1298.)

^d Maximum value at -34°C is given.

^e JP-5 also allows D5972.

^f JP-8 also allows D5972, D7153, and D7154.

^g JP-5: D4809 (D3338, D4529); JP-7: D2382, D3338; JP-8: D4809 (D3338, D4529); RP-1/RP-2: D240

^h JP-5: D3701; JP-7: D3701 (D3343); JP-8: D3701 (D3343); RP-1/RP-2: D3343

ⁱ JP-5: D4294 (D1266, D2622, D3120, D5453); JP-7: D4294 (D1266, D2622, D3120); JP-8: D4294 (D129, D1266, D2622, D3120, D5453); RP-1: D5623 (D5453); RP-2: D5623 (D4045)

^j Alternatively, D4952 can be used with result “negative.”

such modeling capabilities will enable more rapid evaluation and adoption of alternative fuels and their blends for existing aircraft systems, and will be useful in the design of practical combustors for next generation fuels.

Successful demonstration of hydrocarbon-fueled hypersonic technology was achieved with a recent flight test of an X-51A Waverider vehicle burning JP-7.¹¹ A principal challenge for high speed flight is effective thermal management, usually involving active fuel cooling of aerodynamically heated vehicle structures. At fuel system temperatures greater than about 540°C (1000°F), cooling ability can be enhanced beyond physical heat capacity through endothermic reactions in the bulk fuel. However, increased cooling performance comes at a cost to vehicle life if carbonaceous deposits form in heat exchanger passages.² Thus, in the context of specifying chemical composition for hypersonic cooling applications, an understanding of chemical makeup as it relates to fuel cracking and deposit formation is necessary. Compositional requirements for future scramjet and combined cycle systems must account for the interrelated nature of composition and properties, especially for single-fuel applications.

Recent awareness of the potential for chemically unique fuels to impact liquid rocket engine performance motivates an assessment of the variation of currently supplied fuels.¹² Kerosene propellants used in liquid rocket engines are subject to chemical variability due to the intrinsic complexity of petroleum sources as well as subsequent refining to arrive at desired distillate fractions. Blending multiple hydrocarbon fractions to obtain a composition which conforms to specification requirements introduces additional compositional variation. Fluctuating supply and

availability of source materials and differences in production route between suppliers may result in products possessing inherent variability in chemical makeup from one fuel production to another. For decades, LOX-kerosene engines have enabled reliable space launch with an established and relatively stable RP-1 specification. However, technology development for high performance staged combustion systems places more emphasis on non-fluctuating fuel composition, especially when demanding engine performance (Isp) and lifecycle (reusability, operability) goals require fuel operation in environments outside the current experience base.^{13, 14} The need to reexamine the MIL-spec has been raised as a current issue, with an eye toward assessing its suitability in defining kerosene for future launch systems. As with aircraft, clarifying the relationship between fuel composition and behavior in a predictive way is necessary to maximize fuel performance and enable engine design efforts.

III. Variability in Fuel Chemical Composition

A. Composition and Variability of Current Aerospace Fuels

Conventional petroleum-derived jet fuel is the most broadly specified fuel. The density range for JP-8 (and Jet A as specified in ASTM D1655¹⁵) is greater than that of RP-1 by a factor of four. JP-8 specification properties are measured for each batch procured by the Defense Energy Support Center (DESC) and published annually in the Petroleum Quality Information System (PQIS).¹⁶ The report summarizes procurement quantities and specification properties for several product grades and includes statistics (historical trends, geographical region, number of analyses, minimum, maximum, mean, and weighted mean values) useful for assessing fuel variability. The only hydrocarbon composition quantity measured is total aromatic compounds, which for JP-8 was at a weighted mean of 17.92 vol% in 2008. Describing fuel composition by hydrocarbon type distribution is a practical approach for comparing complex kerosenes, particularly since performance is often related to compound classes rather than particular species.^{3, 17} Furthermore, the recent introduction of hydrocarbon class requirements in fuel specifications (cycloparaffin content is limited to 15% by volume for Fischer-Tropsch synthetic paraffinic kerosene blendstocks in jet fuel¹⁸) leads to increased relevance of compositional descriptions via compound type.

The 2006 World Fuel Sampling Program collected 54 fuel samples (JP-8, Jet A, Jet A-1) worldwide,¹⁹ compiling numerous property and performance data which included fuel compositional analysis by hydrocarbon class according to ASTM D2425. Details on this method and discussion of alternative techniques are given in Ref. 20. Table 2 presents the D2425 survey results for JP-8 (10 samples) along with the survey average; an assessment of aromatic and saturate content using ASTM D6379 is also given. The Table 2 results differ somewhat from the

Table 2. Typical Hydrocarbon Class Composition Comparison of Current Aerospace Fuels

Hydrocarbon Type	World Survey Avg. Jet A, Jet A-1, JP-8	Composite Jet A Blend POSF-4658	JP-8 n = 10	JP-5 n = 2	JP-7 POSF-3327	RP-1 POSF-4572
ASTM D2425 ^a , vol %						
Paraffins (<i>n</i> - + <i>iso</i> -)	53	48	54	41	59	49
Cycloparaffins (nc) ^b	19	26	18	22	31	36
Dicycloparaffins (c) ^b	8	6	7	12	8	11
Tricycloparaffins (c) ^b	1	<1	2	2	<1	2
Alkylbenzenes	13	13	14	12	0.7	2.4
Indans + Tetralins	4.6	4.6	4.8	6.7	<0.5	<0.5
Indenes + C _n H _{2n-10}	<0.5	<0.5	<0.5	0.7	<0.5	<0.5
Naphthalene	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
Substituted Naphthalenes	1.6	1.4	1.6	2.8	<0.5	<0.5
ASTM D6379-HPLC, vol %						
Mono-aromatics	18.1	17.5	19.1	19.2	0.9	2.8
Di-aromatics	1.9	1.6	1.9	3.2	<0.1	0.7
Total Aromatics	19.9	19.1	21.0	22.4	0.9	3.5
Total Saturates	80.1	80.9	79.0	77.6	99.1	96.5

Notes:

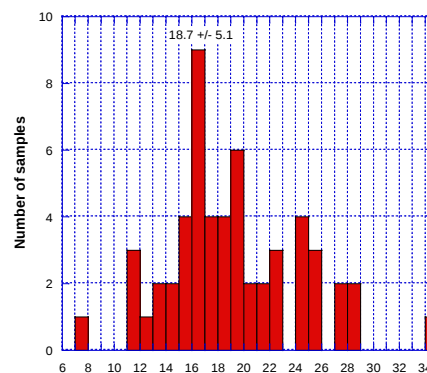
^a The technique also measures acenaphthenes, acenaphthylenes, and tricyclic aromatics, but these were below detection limits in all cases.

^b nc denotes non-condensed; c denotes condensed.

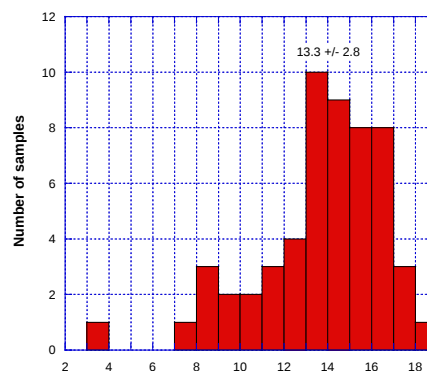
originally-published data for the World Fuel Survey; an improved method for distinguishing between the iso-paraffins and cycloparaffins was used in Table 2. In addition to the world survey results, a composite Jet A fuel (POSF-4658) is included; it was blended from five fuels which were obtained from different manufacturers, and therefore represents an average Jet A composition. JP-5 (2 samples) results are provided for completeness. Results for two specialty fuels (JP-7 and RP-1) demonstrate compositional differences indicative of specification property requirements. The very low sulfur feedstocks used in the production of these blended fuels are also relatively low in aromatic compounds, possibly due to hydrogenolysis of source distillate fractions to obtain high-purity products. The result is much lower quantities of alkylbenzenes and substituted naphthalenes for JP-7 and RP-1 compared with jet fuels. Overall similarities are seen for the various fuels, with compositional discrepancies accounting for the required specifications as discussed previously.

Aside from compositional differences between fuels for specific applications, batch-to-batch variation exists for various reasons. Jet fuel is manufactured in billions of gallons every year in a number of refineries which can produce varying compositions throughout the year depending upon refinery operating parameters and crude oil properties. As shown in Fig. 1, the composition of jet fuel (JP-8, Jet A, Jet A-1) is fairly widely variable. Awareness of the compositional variability for jet fuels is important for developing representative models which will be used to predict properties and performance of candidate alternative fuel blendstocks.

RP-1 is produced in a significantly smaller average annual volume (245,000 gal/yr., 1999-2009) relative to JP-8 (2.7 billion gal/yr., 1999-2008) and is currently not subject to compositional variability due to, for example, operational differences between refineries. Also, the tighter specification requirements for RP-1 limit the extent of variation. However, although the range of compositional variability observed for JP-8 is not expected for RP-1, manufacturing process changes and fluctuating feedstock availability can cause subtle compositional variation which may cause concern for some applications. Whether or not these changes are consequential from an engine or vehicle standpoint depends on the system. Maintaining fuel integrity is universally important for launch applications since vehicle and payload development time and cost are invaluable, especially for manned missions. For the development of new engines, reexamination of the variability in fuel composition, and especially its impact on properties and performance, is in order. Table 3 summarizes literature



a. Cycloparaffins, mass%



b. Alkylbenzenes, mass%

Figure 1. Hydrocarbon class variability from World Jet Fuel Survey

Table 3. Reported RP-1 Hydrocarbon Class Composition

Hydrocarbon Type	Source / Method				
	Ref. 21	Ref. 22	Ref. 3		D2425
Paraffins	vol %	vol %	wt %	vol %	vol %
<i>n</i> -			2.1		7
<i>iso</i> -			27.1		42
Total Paraffins	39	42	29.2	39	49
Cyclics					
Cycloparaffins (nc) ^c	41	25	36.3		36
Dicycloparaffins (c) ^c	14	20	22.3		11
Tricycloparaffins (c) ^c	3	4	3.8		2
Total Cyclics	58	49	62.4	58	49
Aromatics					
Alkylbenzenes		3.1			2.4
Indans + Tetralins		1.7			<0.5
Naphthalene		0			<0.5
Naphthalenes		4.2			<0.5
Total Aromatics	3 ^a	9	8.4 ^b	3	3.5 ^d

Notes:

^a Reported as: Total Aromatics/Detectable Naphthalene (2.00/1.50)

^b ASTM D1319 analysis gives 2.3 vol% total aromatics.

^c nc denotes non-condensed; c denotes condensed.

^d Obtained with ASTM D6379.

references for RP-1 hydrocarbon class composition,^{3, 21-22} including the RP-1 (POSF 4572) composition listed in Table 2 for comparison. While the results shown are subject to analytical differences and span several years, discrepancies are noted. The low production rate of RP-1 hinders our ability to conduct a “world survey” for rocket kerosene. Instead, for the current effort we rely on a set of fuels intended to possess chemical variation which could be correlated with fuel properties and performance.

B. Lab-Scale RP-1 Blends for Compositional Variability Effort

In response to increased awareness of the existing and potential variability of rocket grade kerosene and its importance to operational and developmental systems, several chemically-unique lab scale RP-1 blends were obtained in cooperation with a specialty fuel producer (Haltermann Products). This fuel is currently manufactured by blending hydrocarbon mixtures, or feedstocks, to obtain a product conforming to the MIL-spec as discussed above. Ten formulations were selected for scale-up (~20L) from twelve original hand blends (~1L) based on general composition and preliminary physical property measurements. To provide a frame of reference, the current RP-1 (XC2521HW10) and RP-2 (XK1621HW10) production blend formulations were also supplied. Qualitative blend compositions are shown in Table 4. RP-1 blends manufactured specifically for this effort are denoted “LB...” to identify lab blend as opposed to production batch. Each formulation was produced from an explicit “recipe” of feedstock materials, the proportions of which were not made available. The only imposed criterion was MIL-spec conformance (along with the assertion that the blends are orthogonal, i.e., each blend is formulated from a unique set of feedstocks, and the request that the formulations span total allowable sulfur levels). Therefore, this approach probably does not include the full range of chemical variation resulting from alternative sources or production methods, but represents the variation encountered in as-supplied RP-1 over the past several years and expected in the near future. Given the sensitivity of fuel properties such as volatility to slight changes in chemical makeup, it is uncertain if deviating far from the current formulation would result in a fuel meeting current conformance requirements. Parallel efforts are underway in exploring a wider range of chemical variation than we investigate here, which will guide efforts in fuel specification via hydrocarbon compound classes. Both activities will expand the knowledgebase for future fuel composition optimization.

Table 4. Feedstock Comparison for RP-1 Lab Blends

Blend Name	Feedstock Name								
	A	B	C	D	E	F	G	H	I
LB073009-01			x		x	x			
LB073009-02	x		x		x				
LB073009-03		x	x						
LB073009-05	x	x							
LB073009-06		x		x		x			
LB073009-08	x	x		x					
LB073009-09			x						x
LB073009-10			x		x				
LB080409-01		x					x		
LB080409-05		x						x	

C. Variability in Chemical Composition of Lab-Scale RP-1 Blends

The twelve RP fuels described above were analyzed with ASTM D2425 to obtain hydrocarbon class description and thereby provide a compositional baseline by which to assess fuel property behavior. This method distinguishes between major hydrocarbon types found in aerospace kerosene fuels. Supplemental *n*-paraffin analysis allowed further categorization, with *iso*-paraffin content assumed by subtraction. The results of these efforts are presented in Fig. 2, with mass % hydrocarbon class represented for each sample. In this figure, “aromatics” represents the total of alkylbenzenes, indans + tetralins, and substituted naphthalenes. Five other compound classes are identified but were below detection limits and are therefore not included: indenenes (C_nH_{2n-10}), naphthalene, acenaphthenes, acenaphthylenes, and tricyclic aromatics. Three blends contained measureable aromatic content (all 3.2 mass%). This was a result of our request that at least some formulations be near the “upper rail” on sulfur content, and was accomplished through the use of Feedstock A, a high aromatic, high sulfur, paraffinic solvent used in these three. Total aromatic content was also measured by ASTM D6379, and results were in agreement with D2425 results. As indicated, current RP fuels contain very low levels of aromatics and *n*-paraffins, appreciable quantities of *iso*-paraffins, and typically >50% (mass) combined (i.e. condensed and non-condensed) cycloparaffins.

Since these blends represent the ability of the producer to change fuel composition by varying feedstock selection, we can reasonably suggest an “average” composition for RP-1 (and RP-2, noting the nearly identical compositions of XC2521HW10 and XK1621HW10). Based on current results, Table 5 provides a hydrocarbon class description of as-supplied RP fuels. It should be noted that this average composition does not reflect historical processing differences or fluctuations, as the lab blends herein were provided specifically for this effort. Nor is the producer constrained to an individual feedstock combination, provided the supplied product meets the spec. Also, this composition should not be viewed as average in the sense that all formulations have equal likelihood of use.

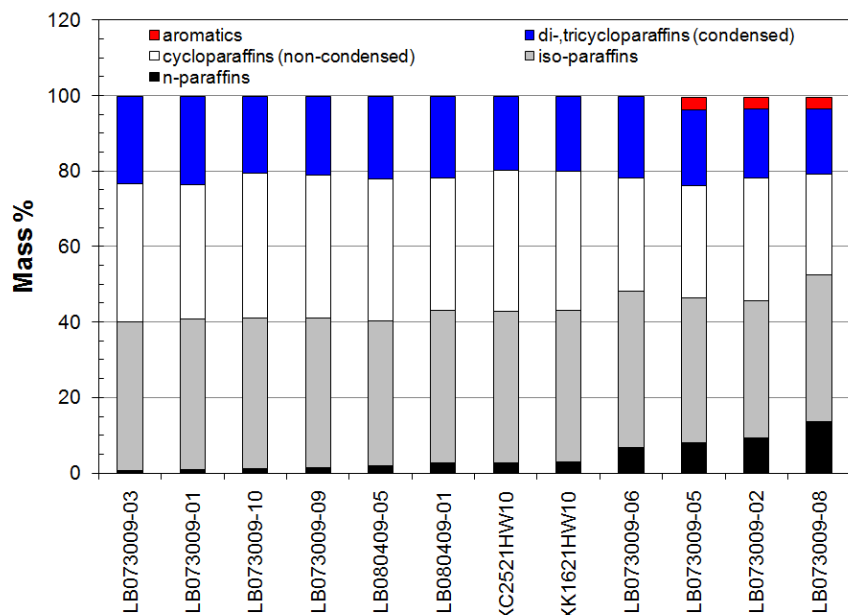


Figure 2. Hydrocarbon class composition of several rocket kerosene batches, obtained by ASTM D2425, D6379, and *n*-paraffin analyses

**Table 5. Average RP-1/
RP-2 Class Composition**

Hydrocarbon Type	Mass %
Paraffins	
<i>n</i> -	5
<i>iso</i> -	39
Total	44
Cycloparaffins	
Cycloparaffins (nc) ^b	34
Dicycloparaffins (c) ^b	17
Tricycloparaffins (c) ^b	4
Total	55
Aromatics	
Alkylbenzenes	0.5
Indans + Tetralins	<0.5
Naphthalene	<0.5
Naphthalenes	0.5
Total	1^a

Notes:

^a Measured up to 4%.

^b nc: non-condensed

c: condensed

Rather, the blend chosen for production depends on transient factors such as source material cost and availability. Therefore, this composition should be used as a guideline rather than a definition of RP-1 composition. Comparing with Tables 2 and 3, it is clear that rocket kerosenes contain consistently high quantities of cycloparaffins, presumably to meet the relatively high density requirement. On the other hand, the low levels of aromatics and *n*-

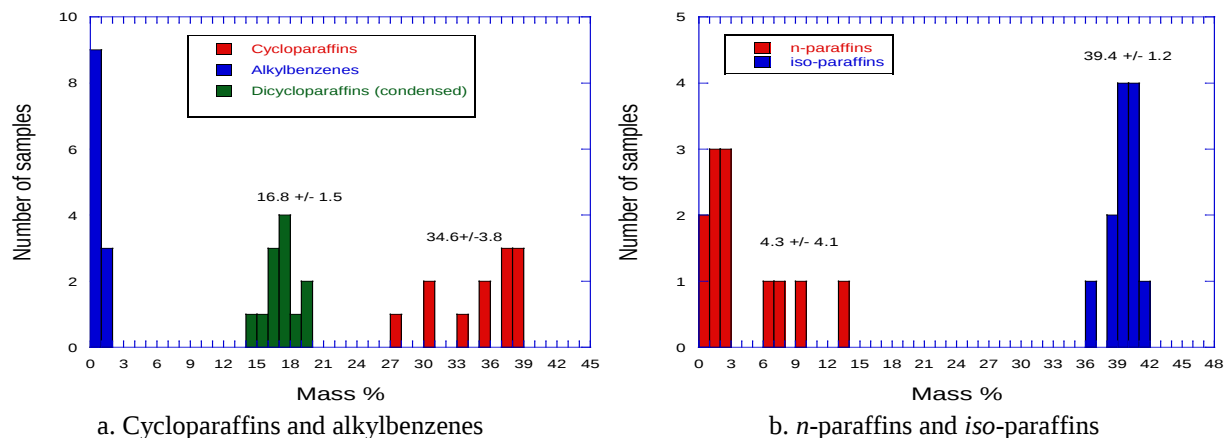


Figure 3. Hydrocarbon class variability for twelve rocket kerosene samples

paraffins in the RP-1 samples are notable compared to jet fuels, which contain roughly 20% of both. As shown in Fig. 3, the compositional variations in RP-1 samples were significantly less than seen in jet fuel. The extent to which this variability influences properties is the subject of the remainder of this paper.

IV. Compositional Effects on Specification Properties and Performance

A. Selection of Appropriate Fuel Properties

The impact of chemical composition on fuel physical properties has been widely demonstrated. In early work describing the motivation for specifying fuels in terms of hydrocarbon composition, Cookson, et al. obtained several composition-property relationships based on multiple linear regression analyses with HPLC and either GC or ¹³C

NMR procedures.^{23, 24} Subsequently, compositional analyses by ^{13}C NMR alone were shown to result in reliable models of multiple jet and diesel fuel properties.²⁵ Later, Cookson, et al. included the effects of boiling range as it influences fuel properties.²⁶ Recently, Liu, et al. demonstrated improved model correlation based on neural network approaches accounting for hydrocarbon classes, boiling range, and several specification properties of eighty jet fuels.²⁷ Liu, et al. then applied these composition-property data to the theoretical design of thermally-stable jet fuel by accounting for carbon deposit as an index of thermal stability, and proposed an optimal composition based on *n*-paraffin, *iso*-paraffin, cycloparaffin, and aromatic content.²⁸ The impact of fuel composition is not limited to specification-defined properties measured with standard methods. Often, application-specific performance requirements demand improved understanding of the role of fuel chemistry in processes such as lubrication, regenerative cooling, atomization, and combustion.²⁸⁻³⁰ The common prospect for these efforts has been identifying the roles of specific fuel constituents or classes on fuel properties, with an eye toward screening potential sources for special-purpose fuels or tailoring fuel specifications to meet the demands of a chosen application or requirement.

It is not a trivial task to determine which property measurements are most important for fuel characterization. This is because properties have many end uses, some of which are property model development, some of which are operational or safety-related, and still others might be regulatory. An approach that allows for property modeling is the most general, since if a model represents a suite of properties, calculations can be done over a range of conditions that are of interest. The end use of property data is key in the selection of which among the myriad of properties are the most descriptive and versatile in achieving the end goal. We opine that a decision must be based on sound technical reasons and should not be restricted to convenience or tradition. A necessary aspect of this philosophy is the consideration and use of new approaches to property characterization. Given the diversification of existing fuel sources, along with operating environments increasingly outside the realm of current experience, the use of modern and developing metrology, albeit nontraditional, is a natural transition.

B. Advanced Distillation Curve

An example of a new approach is the NIST-developed advanced distillation curve (ADC) metrology, also called the composition explicit distillation curve technique. This method is a significant improvement over current approaches, featuring (1) a composition explicit data channel for each distillate fraction (for both qualitative and quantitative analysis); (2) temperature measurements that are true thermodynamic state points that can be modeled with an equation of state; (3) temperature, volume and pressure measurements of low uncertainty suitable for equation of state 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 fraction; and (7) a corrosivity assessment of each distillate fraction. The very significant advantage offered by the approach discussed in this paper is the ability to model the distillation curve resulting from our metrology with equation of state based models. Such thermodynamic model development is

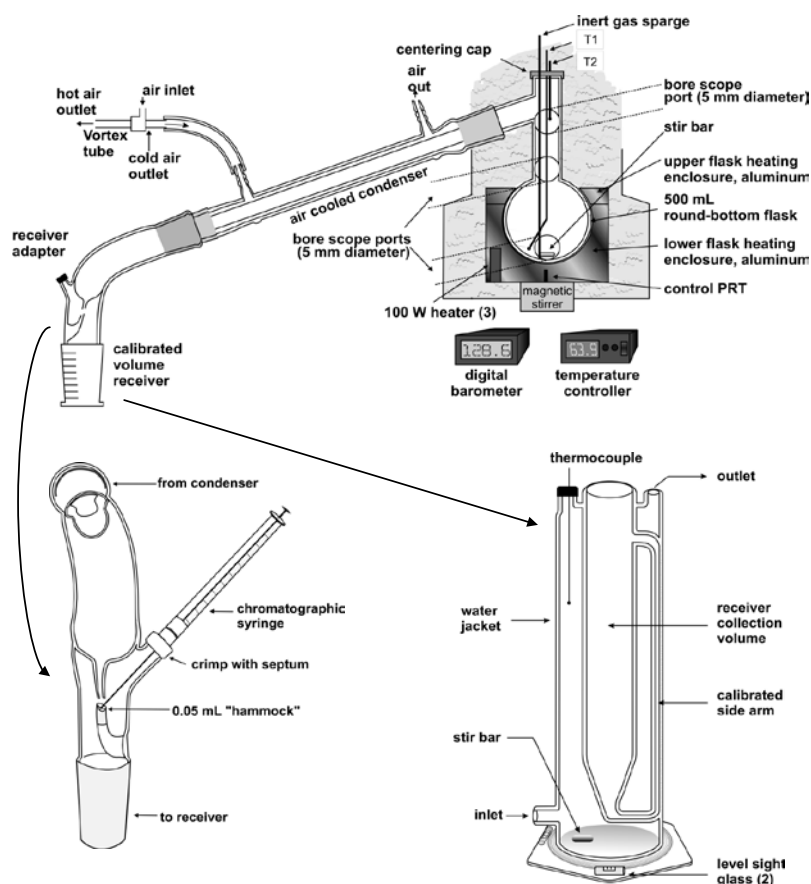


Figure 4. Schematic diagram of the ADC measurement apparatus. Expanded views of the sampling adapter and the stabilized receiver are shown in the lower half of the figure.

simply impossible with the classical approach to distillation curve measurement, or with any of the other techniques that are used to assess fuel volatility or vapor liquid equilibrium. We have applied this metrology to gasolines, diesel fuels, aviation fuels, and rocket propellants.

The method and apparatus for the distillation curve measurement has been reviewed in a number of sources,³¹⁻³⁵ so only a general description is provided here. The required volume of fluid for the distillation curve measurement (in each case, 200 mL) is placed into the boiling flask. Thermocouples are then inserted into the proper locations to monitor T_k , the temperature in the fluid and T_b , the temperature at the bottom of the take-off position in the distillation head. Enclosure heating is then commenced with a four-step program based upon a previously measured distillation curve. This program is designed to impose a heating profile on the enclosure that leads the fluid temperature by approximately 20°C. Volume measurements are made in the level-stabilized receiver, and sample aliquots are collected at the receiver adapter hammock. We typically perform between four and six complete distillation curve measurements for each fluid sample. Figure 4 shows a schematic of the ADC apparatus.

Since the measurements of the distillation curves were performed at ambient atmospheric pressure (measured with an electronic barometer), temperature readings are corrected for what should be obtained at standard atmospheric pressure (1 atm = 101.325 kPa). This adjustment is done with the modified Sydney Young equation, in which the constant term was assigned a value of 0.000109. This value corresponds to the appropriate carbon chain. The magnitude of the correction is of course dependent upon the extent of departure from standard atmospheric pressure. The location of the laboratory in which the measurements reported herein were performed is approximately 1650 m above sea level, resulting in a typical temperature adjustment of 7-8°C. The actual measured temperatures are easily recovered from the Sydney Young equation at each measured atmospheric pressure.

The distillation curve data for thirteen RP samples are presented graphically in Fig. 5. These include ten RP-1 lab blends, the current production formulations for RP-1 and RP-2, and RP-1 sample designated “POSF 4572,” upon which the REFPROP model was formulated. Note that the data are presented in terms of the kettle temperature T_k as opposed to the temperature at the bottom of the takeoff position in the distillation head, and therefore MIL-spec conformance is not indicated. (Specification conformance reports provided with all samples confirmed that ASTM D86 distillation requirements were met.) Since this set of fuels was intended to be chemically unique, the variability in distillation behavior is not surprising, especially given its sensitivity to composition. In these samples, fuel

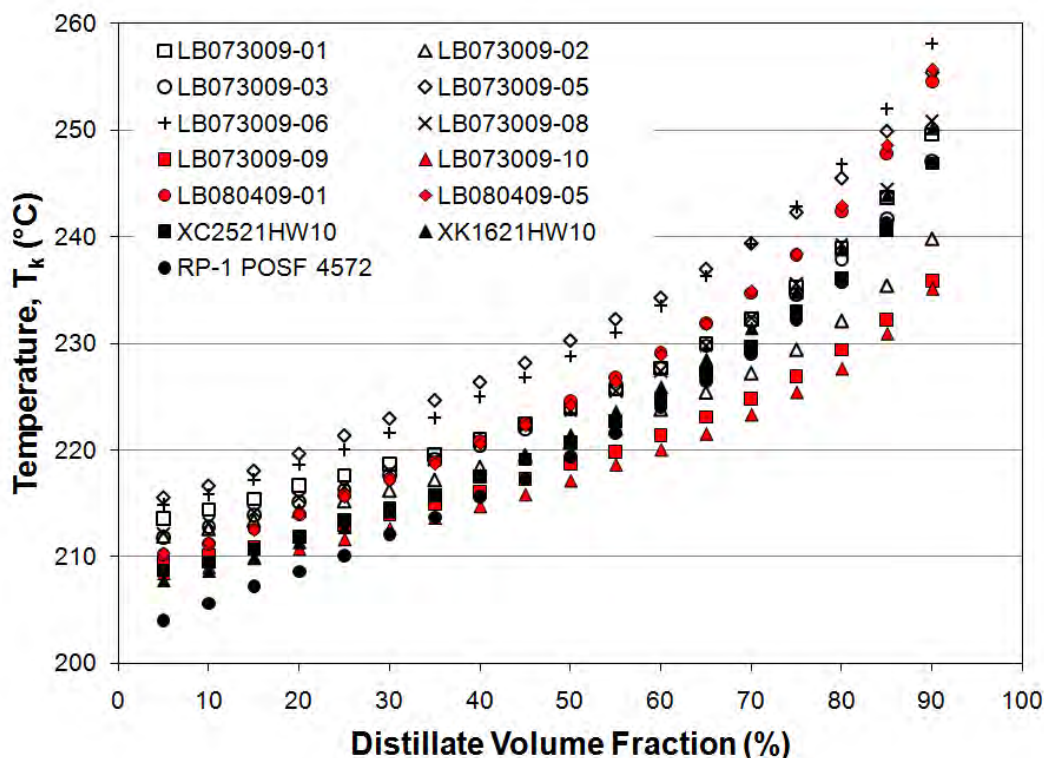


Figure 5. Distillation curves obtained by ADC method of ten lab blend RP-1 samples, current production RP-1 and RP-2, and the RP-1 sample used to develop the REFPROP model (POSF 4572)

composition is shown to influence both the overall volatility (compare LB073009-06 and LB073009-10) as well as the distillation curve profile (compare LB073009-02 and LB080409-05). LB073009-09 and LB073009-10 exhibit consistently low boiling temperatures throughout the distillation due to the abundance of low molecular weight compounds (monocyclo-paraffins) as shown in Fig. 2. Additionally, these blends have the lowest 90% distillation temperature, an effect of the relatively low molecular weights of the final eluting compounds. (The greatest molecular weight compounds identified in LB073009-10 and LB073009-06 were 4,6-dimethyl-dodecane, 198.3880 M.W.; and 2,6,10,14-tetramethyl-pentadecane, 268.5209 M.W., respectively.) Another important consideration is behavior of the distillation curve based on sample POSF 4572. This curve possesses both lower initial distillation temperatures as well as a different overall profile as compared with several lab blends produced for this study. On closer examination, the shape of the distillation profile is very similar to those of other blends, particularly LB080409-01 and LB080409-05, although the downward offset is of concern and may be a consequence of a unique feedstock used in the production of POSF 4572 which was not present in the current lab blends. It should be noted that the current REFPROP model is based on POSF 4572 and closely predicts the distillation behavior of that batch.³⁶ However, it is expected that volatility of as-supplied rocket kerosene is slightly overestimated.

C. Density and Viscosity

Fuel density as measured with a Parr DMA48 density meter in accordance with ASTM D4052-96 are given Fig. 6. For clarity, only five rocket kerosene samples from the current work are shown: LB073009-01, LB073009-05, LB073009-08, XC2521HW10, and XK1621HW10. These represent the maximum (absolute), maximum (in-spec), minimum, current RP-1 production, and current RP-2 production, respectively. Additionally, density at 15°C (60°F) of a recent RP-1 production, WD2521HW02, was provided by the fuel producer and is shown for reference. This batch possessed an abnormally low density compared with production fuel at that time, although it clearly meets specification requirements at 15°C. Also, literature data for RP-1 and RP-2 are provided as measured by Outcalt, et al,³⁷ although those measurements were made on different fuel samples. As indicated, the density of blend LB073009-01 (0.816 kg/m³) was outside the allowable range of 0.799-0.815 kg/m³ at 15°C (indicated by gray vertical bar), but is included nonetheless. This was the only occurrence of any delivered lab blend failing to meet

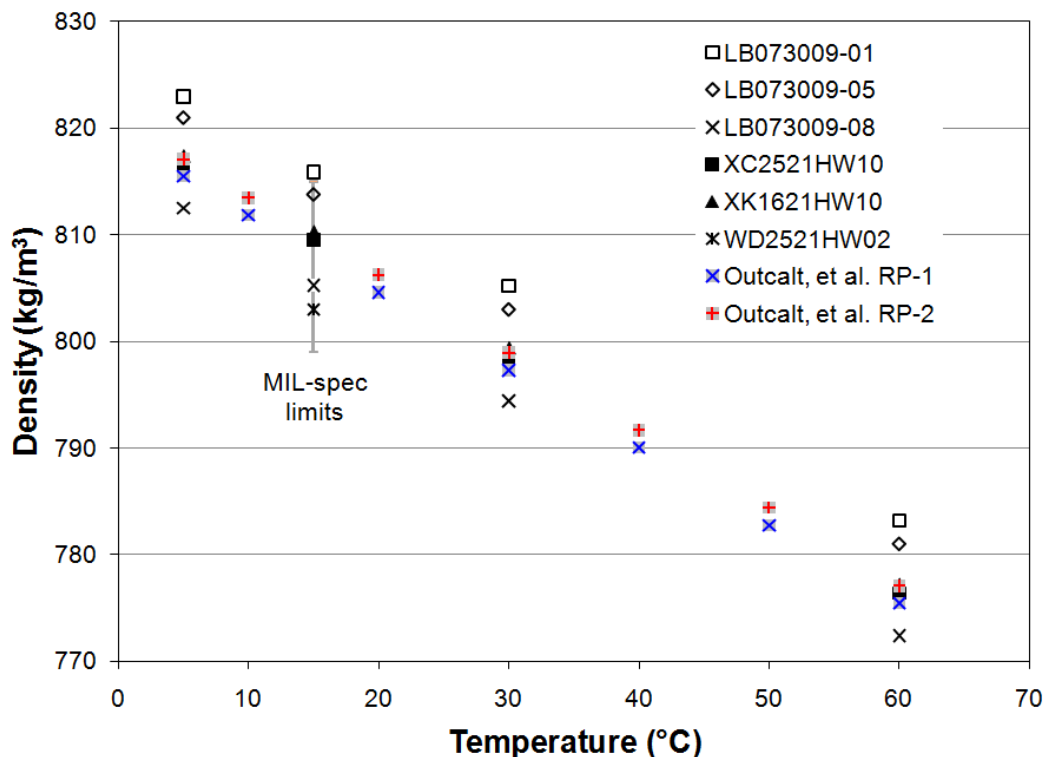


Figure 6. Variation in density for selected RP blends: LB073009-01 (maximum density, absolute), LB073009-05 (maximum density, in-spec), and LB073009-08 (minimum density). Current production RP-1 (XC2521HW10) and RP-2 (XK1621HW10), a recent low-density batch (WD2521HW02), and literature values from Ref. 37 are also provided.

spec, and was attributed to slightly different feedstock proportions during the scale-up to 20L quantities. With the exception of this out-of-spec sample, fuel density for the remaining seven samples is bounded by LB073009-05 and LB073009-08, with all density values for RP-1 lab blends within the upper two-thirds of the allowable range. The density data follow expected behavior in terms of fuel composition; that is, fuels with high relative abundance of multiple ring cycloparaffins and aromatic compounds (e.g. LB073009-01 and LB073009-05, cf. Fig. 2) also have the greatest density. Conversely, LB073009-08 is high in *n*-paraffin content and has the lowest density overall. A more surprising aspect of the density variation depicted here is the apparent sensitivity of density to different feedstocks. Inspection of Table 4 shows that LB073009-05 and LB073009-08, the highest and lowest density blends, differ compositionally only in the presence of Feedstock D in LB073009-08. This indicates that Feedstock D is rich in lower molecular weight *n*-paraffins, which is substantiated by the higher volatility of LB073009-08 compared with LB073009-05 (see Fig. 5); the compositional distribution in Fig. 2, and the greater abundance of C10 – C12 *n*-paraffins which is seen in Fig. 7. It should not be understated that the presence of a single feedstock in a fuel blending operation can result in a density swing of more than half the allowable specification range. This example illustrates the care that must be taken when considering new formulations. It is reasonable to expect that further increases in *n*-paraffins will in turn decrease fuel density. The degree to which fluctuations of this magnitude could be expected to impact system performance remains to be determined. It is likely that sensitivity of variations in composition may be engine- or application-specific,

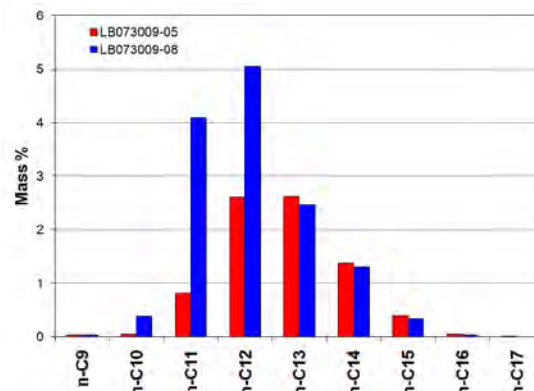


Figure 7. Comparison of *n*-paraffin distribution for RP-1 batches with high (LB073009-05) and low (LB073009-08) measured density

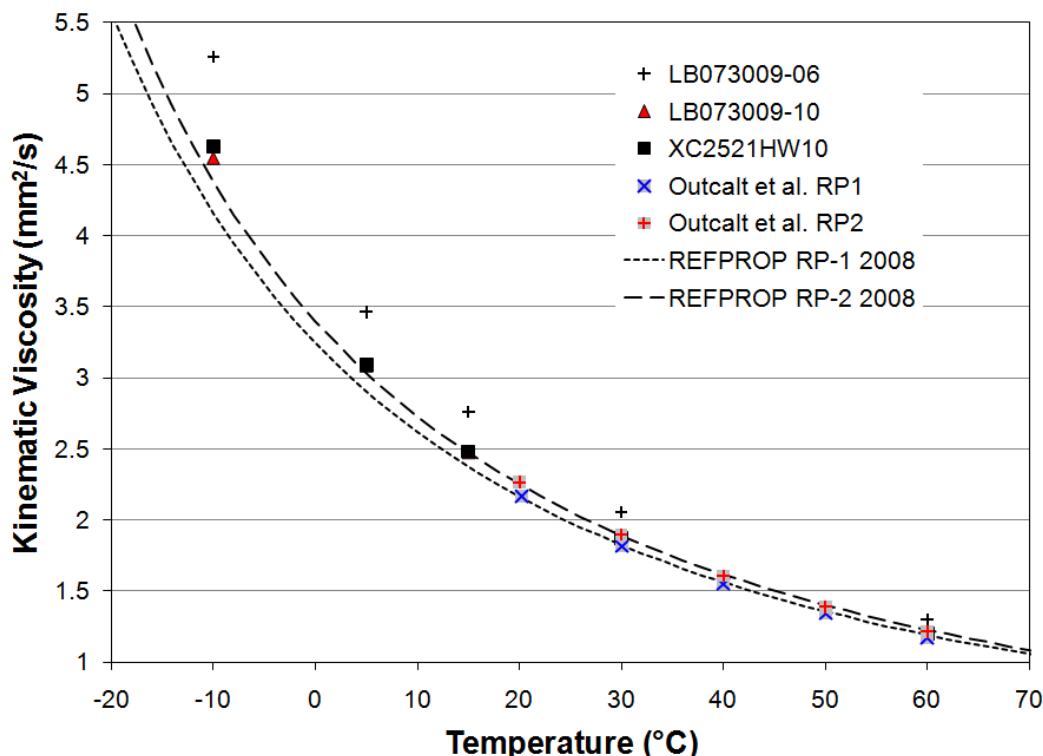


Figure 8. Variation in kinematic viscosity for selected RP blends: LB073009-10 and LB073009-06 span the range of viscosities encountered in fuel blends for this study. XC2521HW10 is the current production RP-1. Experimental values from Ref. 37 and current model predictions (Ref. 38, 39) are also provided.

emphasizing the need to consider the needs of all current and potential fuel users, as well as manufacturers, when embarking on specification development or modification efforts.

Accurate fuel viscosity data is important for the design of multiple components in liquid rocket engines, including regenerative cooling system pressure loss; low-temperature injector flow behavior (fuel in proximity to liquid oxygen); and fuel lubricating ability for rotating components such as bearings. Viscosity of each blend was measured using ASTM D445-01, and results for several fuels are given in Fig. 8 as a function of temperature. Also included are results for the current production RP-1 formulation (XC2521HW10), data obtained by Outcalt, et al.,³⁷ and the current kinematic viscosity predictions for RP-1 and RP-2 obtained by REFPROP.^{38, 39} Viscosity data for other RP-1 blends are spanned by LB073009-10 and LB073009-06 and are not shown. High proportions of high molecular weight *n*- and *iso*-paraffins are expected to result in higher viscosity, while naphthenic and aromatic compounds have an opposing effect. This is evident when examining the composition of LB073009-06, which contains the greatest quantity of paraffins (*n*- and total) of any blend without the high-aromatic Feedstock A.

An important outcome of this collaborative work is to allow REFPROP accommodations for compositional variation. While current models do an excellent job predicting properties of the fuel samples on which they are based (compare experimental data of Outcalt, et al. and REFPROP predictions), the ability to account for deviations in a given fuel composition from REFPROP predictions is desired. Ideally, the REFPROP model will predict the expected mean value of multiple batches. Furthermore, current efforts at the National Institute of Standards and Technology (NIST) are intended to explore the capability of tuning REFPROP output based on a set of appropriate fluid descriptors. This will allow fuel users to make estimates of physical properties, especially useful when formulations fall outside the current experience base, as in the case of 50/50 blends of petroleum-derived and alternative source aviation kerosene. In the lab blends acquired for this study, viscosity appears high compared with currently-supplied RP-1 and the model predictions.

D. Energy Content and Heat of Formation

Heat of combustion is an experimentally-determined indicator of fuel energy content. Along with molar H/C ratio, it is used to calculate enthalpy of formation, a quantity used in theoretical performance predictions for liquid

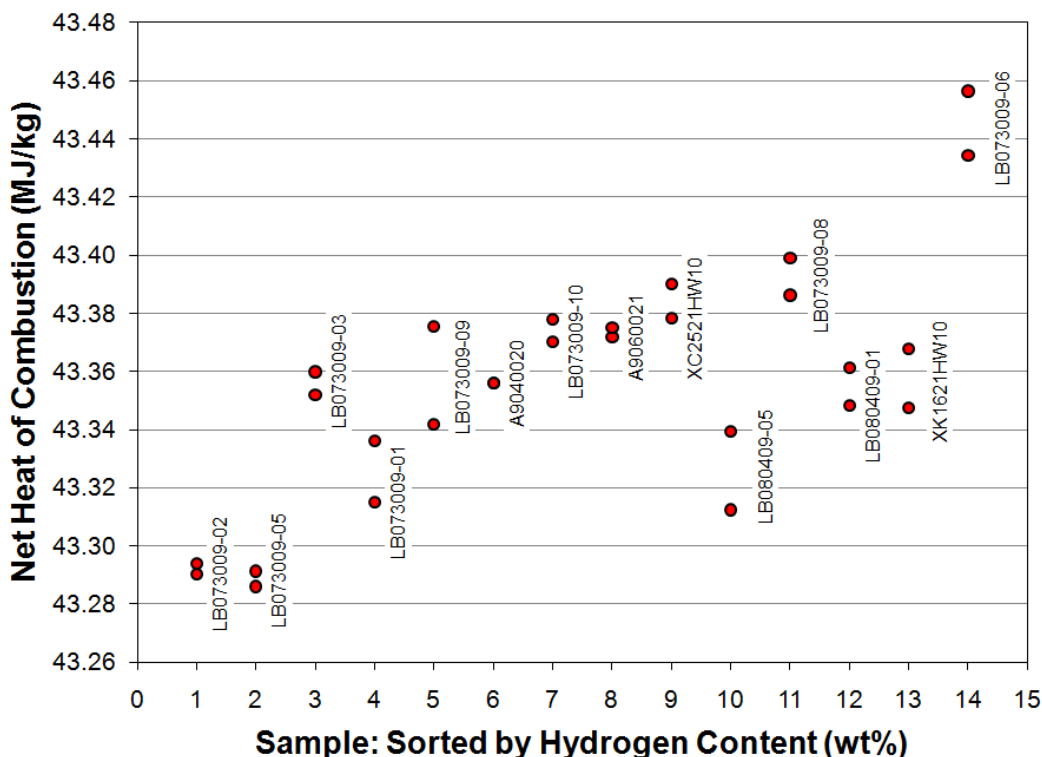


Figure 9. Measured net heat of combustion as a function of hydrogen content for several RP batches. Duplicate heat of combustion data are shown to indicate precision. Results are sorted based on wt% hydrogen (average of two measurements) in ascending order. A9060021 and A9040020 are recent production batches of RP-1 obtained from launch sites.

rocket engines. Different methods are used to guide analytical measurements of net heat of combustion. MIL-DTL-25576E specifies the use of ASTM D240 for RP-1, with minimum allowable net heat of combustion of 18500 Btu/lbm (43 MJ/kg). Net heat of combustion was measured using an isoperibol calorimeter following ASTM D4809; results on a mass basis are shown in Fig. 9 for fourteen fuels including ten RP-1 lab blends, the current formulations for RP-1 and RP-2, and two recent RP-1 production batches obtained from launch locations. Duplicate measurements were taken for each RP sample; both are shown to indicate the precision of the method. The heat of combustion data are plotted against average measured hydrogen wt% for each sample, measured in duplicate with a Perkin Elmer Elemental Analyzer (Model EA2400). Hydrogen content for the fourteen samples shown ranged from 14.1 to 14.4 wt% (mean 14.30 wt%). Fuel with high levels of cycloparaffins and aromatics and similar average molecular weights are expected to demonstrate low energy (mass basis) and hydrogen content, while the opposite is true for fuels with high concentrations of *n*-paraffins. In general, this behavior is demonstrated in the data. Since heat of combustion is dependent on molecular weight and compound class, correlating energy content behavior with composition for complex mixtures of similar chemical makeup is challenging. However, it is noteworthy that LB073009-06, with the greatest hydrogen content and also the greatest net heat of combustion, is also the blend with the highest level of paraffins (*n*- and total) with simultaneous low aromatic content. On the other hand, LB073009-05 and LB073009-02, with relatively high levels of aromatics exhibit both low heat of combustion and low hydrogen content.

V. Conclusion

In this paper we have reintroduced the motivation for (1) developing relationships between fuel composition and physical properties and performance; and (2) incorporating these models in the optimization of fuel composition to meet future engine and vehicle system requirements. Multiple aerospace propulsion and energy applications stand to benefit from outcomes of this effort, and a collaborative approach is therefore ideal. Current engine development activities prompt an assessment of as-supplied rocket kerosene, the set of requirements used for its specification, and the potential impacts compositional variations have on engine operability and performance. To address the present need within the scope of future fuel development and specification efforts, we obtained several chemically unique RP-1 formulations from a specialty fuel manufacturer. These blends were intentionally orthogonal (produced from unique sets of feedstocks) and represent the expected variation in composition of currently produced RP-1. Chemical composition was obtained in terms of hydrocarbon types and was compared between the various formulations. Several property measurements provided insight to compositional impacts on fuel behavior; reported in this paper are composition explicit distillation curve, density, viscosity, heat of combustion, and hydrogen content. While chemical variability for RP-1 was not as extensive as that of jet fuel, the sensitivity of several properties to feedstock selection was demonstrated, even for fuels which met specification requirements. Therefore we conclude that compositional variability is consequential from an engine design perspective, and expanded properties and performance data (such as lubricity and thermal decomposition) are necessary for gauging operational impacts and for informing future fuel and specification development efforts.

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