Effect of RP-1 Compositional Variability on Thermophysical Properties

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In this paper we compare experimental and calculated thermophysical properties of two samples of rocket propellant RP-1 obtained from different batches of RP-1 that exhibit compositional variations. One sample is atypical, due to a high olefin content. The effect of the compositional variation is shown for several thermophysical properties such as density, sound speed, viscosity, thermal conductivity, and the volatility (as expressed by the distillation curve). We also compare two different surrogate mixture models that were developed for each fuel sample. The greatest effects of this significant compositional variability are seen in the viscosity and the distillation curve.

Introduction

Modern rocket motors can operate on either a liquid or a solid fuel package, although the liquid fuel package is the more easily controlled and the more flexible of these two classifications.[1] Indeed, Goddard's initial 1926 rocket flight tests used a liquid fuel package consisting of oxygen and gasoline. Since that time, the major practical liquid fuel packages have been those based either on liquid oxygen + alcohol/water, oxygen + hydrogen, or oxygen + kerosene.[2,3] Although the oxygen + hydrogen mixture is the highest performing practical propellant mixture commonly used in terms of specific impulse (actually, hydrogen + fluorine is higher, but is clearly not practical), it has significant limitations that include the complexity and cost of cryogen use (with temperatures near 20 K), the hazards associated with liquid hydrogen, and very low energy density (when compared to a hydrocarbon mixture such as kerosene). The initial oxygen + kerosene propellant mixtures that were developed utilized turbine aviation fuels as the kerosene component, starting with the kerosene-like fluid JP-4. The aviation fuels were not produced with a sufficiently tight set of specifications (in terms of physical properties such as density, volatility, chemical components, enthalpy of combustion, etc.) to be effective rocket propellants, however.

This limitation led to the development of RP-1 (for rocket propellant 1) in the mid 1950s. This fluid, produced as MIL-P-25576, has a much tighter allowable density and volatility range, and a much lower sulfur, olefin, and aromatic content than those of the common turbine aviation fuels.[4] RP-1 is now a long-established hydrocarbon fuel that continues to be widely used in propulsion systems. Distillates from crude oil that are high in naphthene content are generally used for RP-1 production in order to meet the specifications for density, heat of combustion, and aromatic content. Previous analysis of RP-1 has shown the fuel to be a complex mixture of compounds including paraffins, olefins, and aromatics. Although the sulfur concentration specification for RP-1 was set at 500 ppm (mass/mass), the typical as-delivered lot was much lower, at 30 ppm (mass/mass).[5]

The desire in recent years to use rocket motors many times, rather than a single time, has led to reformulations of the kerosene component of liquid rocket propellants. In terms of processing, increased hydrotreating of fluids such as RP-1 can lower the sulfur, olefin, and aromatic content significantly. The resulting fuels have demonstrably lower metal corrosion and erosion effects, and are thus more amenable to multiple-use rocket motors. Three grades of RP-1 were later specified with the ultimate goal of decreasing the sulfur concentration specification: TS-30 (with a total sulfur specification < 30 ppm, mass/mass, which was similar to that of a typical as-delivered RP-1), TS-5 (total sulfur specification of < 5 ppm, mass/mass), and UL (ultralow sulfur, < 100 ppb, mass/mass). Testing showed that ultralow sulfur RP-1 provided significant performance benefits over TS-5 with only marginally greater costs, so this fluid (ultralow) was selected to become what is now called "RP-2". The RP-1 sulfur limit was lowered from 500 to 30 ppm (mass/mass), more closely reflecting the typical as-delivered material. We note that the specification for RP-1 and RP-2 aromatic content are the same, however one commonly finds a lower aromatic content in RP-2.[4,6]

It has become clear that although the specification for RP-1 is relatively tighter than those for large volume fuels, the actual fuels as-delivered may be subject to substantial variation.[7] Moreover, it is not clear that the specifications that currently exist fulfill all needs of system designers and

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Table 1. A Listing of the Major Components Found in RP-1, Sample A

name	CAS No.	RMM	area %
1,3,5-trimethyl cyclohexane	001795−26−2	126.14	0.654
2-methyl decane	006975−98−0	156.19	0.817
2,2-dimethyl butane	000075−83−2	86.11	2.375
3-methyl decane	013151−34−3	156.19	3.985
3-ethyl-4,4-dimethyl-2-pentene	053907−59−8	126.14	2.726
2,9-dimethyl decane	001002−17−1	170.2	6.280
2-methyl-cis-decalin	1000152−47−3	152.16	3.970
decahydro-2-methylnaphthalene	002958−76−1	152.16	2.574
cis-syn-1-methydecalin	1000158−89−1	152.16	4.652
1-hexyl-3-methylcyclopentane	061142−68−5	168.19	5.099
1-dodecene	000112−41−4	168.19	5.995
2-methyl undecane	007045−71−8	170.2	3.124
3-methyl undecane	001002−43−3	170.2	2.839
2,2-dimethyl-decadi-3,5-ene	055638−50−1	166.17	2.735
methylcyclododecane	NA	182.22	3.580
n-dodecane	000112−40−3	170.20	5.327
2,7,10-trimethyl dodecane	074645−98−0	212.25	3.765

Table 2. A Listing of the Major Components Found in RP-1, Sample B

name	CAS No.	RMM	area %
2,6-dimethylnonane	17302−28−2	156.19	1.761
x,y-dipropylcyclopentane	NA	154.17	1.043
l-ethyl- 2-propylcyclohexane	62238−33−9	154.17	0.0461
trans-decahydronaphthalene	493−02−7	138.14	1.402
2-methyldecane	6975−98−0	156.19	1.588
3-methyldecane	13151−34−3	156.19	1.260
n-undecane	1120−21−4	156.19	2.592
2- methyl-trans-decalin	1000152−47−3	152.16	1.355
2,6-dimethyldecane	13150−81−7	170.2	1.242
2-syn- methyldecalin	1000155−85−6	152.16	2.003
1,3-dimethylbutylcyclohexane	61142−19−6	168.19	1.364
5-methylundecane	1632−70−8	170.2	1.693
2-methylundecane	7045−71−8	170.2	2.287
5-ethyldecane	17302−36−2	170.2	1.384
1- methyl-1, 2-pentylcyclohexane	54411−01−7	168.19	1.059
n-dodecane	112−40−3	170.2	2.351
2,6-dimethylundecane	17301−23−4	184.22	1.967
4-methyldodecane	6117−97−1	184.22	1.506
2-methyldodecane	1560−97−0	184.22	1.817
7-methyltridecane	26730−14−3	198.24	1.698
tridecane	629−50−5	184.22	2.585
1- methyl naphthalene	90−12−0	142.08	1.220
6-methyltridecane	13287−21−3	198.24	1.025
2-methyltridecane	1560−96−9	198.24	1.117

operators. For these reasons, it is desirable to evaluate how variability in properties, and in the specifications for those properties, will affect operability. As a first step, we present here an evaluation of the effect of a substantial difference in RP-1 properties on the ability to model such properties with thermodynamic and transport property theory. This substantial difference in properties arose from major compositional variations that were observed between two different samples of RP-1.[6,8] We note that our purpose here is not to determine how widespread such differences might be. This is an important follow-on task, but it is beyond the scope of the present inquiry. Here, we merely use the opportunity of an observed compositional difference to evaluate what effect such a difference might be expected to have on thermodynamic and transport properties and models.

Experimental Section

Two different samples of RP-1 were obtained from the United States Air Force, Air Force Research Laboratory, Propulsion Directorate, and were used without treatment or purification. Care was taken to minimize exposure to the atmosphere to minimize oxidation, evaporation of the more volatile components, and uptake of moisture. One sample, designated as sample A, was later found to be atypical in composition and behavior. The other sample, designated sample B, is representative of rocket kerosenes in terms of composition and properties. Both samples of RP-1 were pink in color because of the presence of a dye, azobenzene-4-azo-2-naphthol. We noted that sample A was significantly darker than sample B, although it is not clear whether this plays any significant role in compositional variability.

The samples A and B were subjected to an extensive chemical analysis in previous work. This work was done with a gas chromatography−mass spectrometry−Fourier transform infrared spectrophotometry method (GC-MS-FTIR, 30 m capillary column of 5% phenyl dimethyl polysiloxane, having a thickness of 1 μm, temperature program from 90 to 250 °C, 10 °C/min). Mass spectra were collected for each peak from 15 to 550 RMM

(relative molecular mass) units, and infrared spectra were collected between 4000 and 600 cm^{-1}.[9,10] The assignment of major components was presented earlier,[11] but a summary of those compositional measurements is provided in Table 1 for sample A and Table 2 for sample B. Some comments regarding the components we identify and subsequently choose for possible inclusion in our surrogate models are in order. First, we include major components that are present in mole percentages in excess of 1%. Then, we make an effort to include some representative heavy components and some representative lighter components. This is critical, since we must have a distribution that covers the entire thermophysical property range in order to develop a useful surrogate model.

As mentioned earlier, the first sample (A) was unusual in that chemical analysis showed a much larger fraction of olefinnic and aromatic compounds than would be expected in a typical rocket kerosene fraction. Approximately 20% of the compounds identified in this mixture had a double bond or an aromatic ring (note that the lists provided in Tables 1 and 2 are not exhaustive). It is therefore representative of what might be considered an off-specification lot of RP-1. The second sample (B) was more typical of a kerosene rocket propellant, with very low olefinnic and aromatic fractions. This sample is considered to be representative of typical as-delivered RP-1, a fluid that has a relatively tighter specification than commodity fuels such as aviation fuel, diesel fuel or gasoline.

In addition to analysis by GC-MS-FTIR, a total sulfur analysis was done on both fluids by gas chromatography with a sulfur chemiluminescence detector (SCD). Moreover, a copper strip corrosion test was done for each. The results of the SCD and copper strip test indicated that both samples were very low in sulfur (less than 30 ppm mass/mass). Detailed analytical results for both fluids are available elsewhere.[6,8,11−14]

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Table 3. Composition of Surrogate Model for RP-1 Sample A

fluid	mole fraction	family	mole fraction
3-ethyl-4,4-dimethyl-2-pentene	0.0998	olefins	0.2664
cyclodecene	0.0212		
1-dodecene	0.0264		
4-methyl-4-undecene	0.1045		
1-tridecene	0.0145		
2-methylnaphthalene	0.051	aromatics	0.051
heptylcyclohexane	0.1422	naphthenes	0.4083
cyclododecane	0.0427		
2-methyldecalin	0.2234		
2-methylnonane	0.0233	paraffins	0.2743
3-methyldecane	0.1084		
dodecane	0.0193		
2,7,10-trimethyldodecane	0.1038		
hexadecane	0.0195		

Table 4. Composition of Surrogate Model for RP-1 Sample B

fluid	mole fraction	family	mole fraction
		olefins	0
		aromatics	0
1-methyldecahydronaphthalene	0.354	naphthenes	0.667
heptylcyclohexane	0.313		
5-methylnonane	0.15	paraffins	0.333
dodecane	0.183		

Thermodynamic and Transport Property Models

In previous work[8,15] two different models for RP-1 were developed; they are summarized in Tables 3 and 4. The models were designed to represent the two different samples of RP-1 described above. RP-1 is a complex mixture of hundreds of components, and modeling each individual constituent is not feasible. We instead developed models based on the concept of a surrogate mixture in which one uses a mixture of a relatively small number of components (usually less than 20) to represent the behavior of the actual complex fuel. Edwards and Maurice[16] reviewed surrogate models for aviation and rocket fuels and provided an overview of the general requirements and expectations of fuel surrogates.

The first model, originally developed in 2003,[8] was based on the atypical RP-1 sample described above, sample A. The surrogate contains 14 components summarized in Table 3. It was developed by fitting experimental densities, heat capacities, thermal conductivities, viscosities, and the initial boiling point (measured at local atmospheric pressure). At the time the model was developed, the advanced distillation curve method[13,17−20] was not yet available. In fact, during this project we realized that in order to develop better surrogate models, a better method of determining the volatility behavior was necessary. This need led to the development of the advanced distillation curve methodology. Comparative calculations based on this earlier model[8] indicated that the model represents the density (over a range of temperatures 274−600 K at pressures to 60.6 MPa) to within 0.3% (at a 95%

confidence level), the heat capacity to within 7%, the thermal conductivity (over a range of temperatures 300−600 K at pressures to 70 MPa) to within 3%, the viscosity (over 243−333 K) to within 3% at atmospheric pressures and 10% at 60 MPa, and the boiling point at local atmospheric pressure to 0.5%. Table 5 gives additional calculated properties of the model. The surrogate mixture used in this model has an overall molar mass of 164.6, a hydrogen to carbon ratio (H/C) of 1.95, and an approximate chemical formula of $C_{11.8}H_{23.0}$. The overall composition is 27.4% alkanes, 26.6% alkenes, 18.5% monocyclic paraffins, 22.4% bicyclic paraffins, and 5.1% aromatics (mol/mol). We emphasize that this composition is not the actual mixture composition, but rather a surrogate mixture that approximates the thermophysical property behavior of the RP-1 sample (A) that was investigated.

A second model, based on the sample of RP-1 designated sample B, was developed more recently.[15] It was formulated by fitting experimental densities, sound speed at atmospheric pressure, thermal conductivities, viscosities, and the advanced distillation curve. The composition of this surrogate mixture is given in Table 4; it contains only the four components α-methyldecalin, 5-methylnonane, n-dodecane, and heptylcyclohexane. Comparative calculations based on this model[15] indicated that the model represents the density (over a range of temperatures 270−470 K at pressures to 40 MPa) to within 0.4%, the speed of sound at atmospheric pressure to within 2%, the thermal conductivity (over a range of temperatures 301−553 K at pressures to 61.7 MPa) to within 4%, the viscosity at atmospheric pressure to within 2%, and the advanced distillation curve to within 0.5%. The surrogate mixture has an overall molar mass of 163.5, a hydrogen to carbon ratio (H/C) of 2.00, and an approximate chemical formula of $C_{11.66}H_{23.32}$. The overall composition is 33.3% alkanes and 66.7% cyclic paraffins (mol/mol); there were no alkenes or aromatics in this surrogate. The net heat of combustion was computed by a mole fraction average of the component enthalpies, ignoring the enthalpy of mixing.[6,21] The constituent heats of combustion were obtained from the DIPPR database.[22] When available, experimental data were used; otherwise the Cardozo method[23] of equivalent chains was utilized. The calculated density, viscosity at −34.4 °C (−30 °F), hydrogen, aromatic and olefin content, and heat of combustion meet the military specifications for RP-1.[24]

Comparisons

To demonstrate the effect of compositional variability of RP-1, we compared calculations of thermophysical properties obtained from the models described above with each other, and with available experimental data.

Figure 1 illustrates the effect of compositional variability on the kinematic viscosity at atmospheric pressure. The data shown for the atypical sample A were measured by use of an open gravitational capillary viscometer (Ubbelohde type glass capillary) and have an estimated uncertainty of 1%; experimental details and a detailed uncertainty analysis are given elsewhere.[8] The data for the more typical sample B

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Table 5. Selected Calculated Characteristics of the Two Surrogate Mixtures Used in the Thermodynamic and Transport Property Models

	RP-1 model, 2003	RP-1 model, 2008
MW	164.6	163.5
formula	$C_{11.8}H_{23.0}$	$C_{11.66}H_{23.32}$
H/C	1.95	2.00
heat of combustion (J/mol)	-7.18×10^6	-7.18×10^6
density[a] at 288.7 K (60 °F) (kg/m^3)	805.3	808.1
speed of sound[a] at 288.7 K (m/s)	1318.5	1330.9
thermal conductivity[a] at 288.7 K (mW/m·K)	114.1	112.76
viscosity[a] at 288.7 K (mPa·s)	1.78	1.90
initial boiling point[a](K)	465.3	475.6
kinematic viscosity[a] at 238.7 K(−30 °F) (cm^2/s)	0.081	0.091
T_c (K)	676	677
p_c (kPa)	2300	2210
ρ_c (kg/m^3)	220	235

[a] At 101.325 kPa.
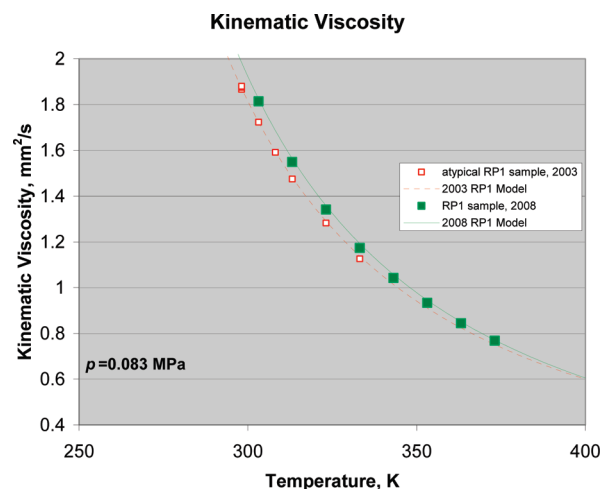
Figure 1. Kinematic Viscosity of RP-1, samples A and B, along with the results from the respective surrogate model.
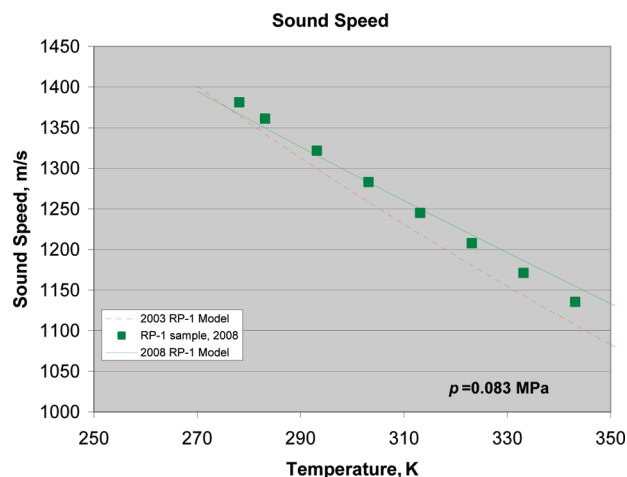
Figure 2. Sound speed of RP-1, sample B, along with the along with the results from the respective surrogate model.

measured recently[25] were also obtained in an automated open gravitational flow viscometer (Ubbelohde type glass capillary) with an estimated uncertainty of 1.5%. The calculated viscosity from the 2003 and the 2008 models[8,15] are also shown. At room temperature, the atypical sample viscosity is about 6%

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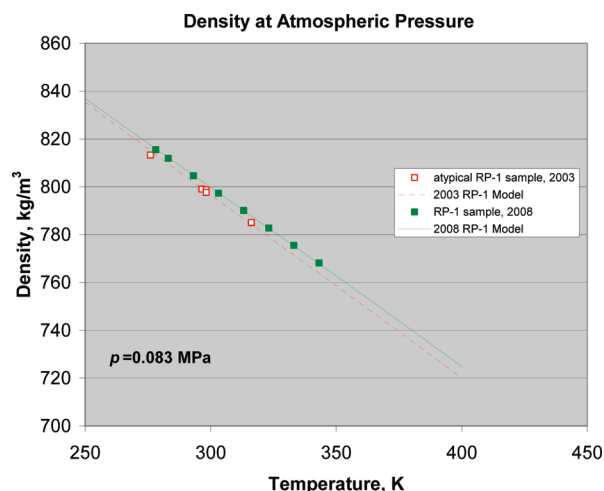
Figure 3. Density at atmospheric pressure of RP-1, samples A and B, along with the results from the respective surrogate model.

higher than that of the typical sample. This difference exceeds the uncertainties of the measurements and the models and represents a significant property variation due to sample variability. Such a difference is significant from an operational standpoint as well.

Figure 2 shows the calculated speed of sound for both models, and experimental data for sample B. The experimental data[25] were obtained by a pulse-echo speed of sound method and have an estimated uncertainty of 0.1%. Experimental data were not available for the atypical sample, so comparisons cannot be made. The values calculated by the models agree with each other at the lowest temperature (270 K) but show slightly different temperature dependencies that result in differences of 4% at 343 K. Data for the speed of sound were not used in the development of the model for sample A and therefore the model is considered totally predictive for this property.

Figure 3 illustrates the model calculations for the density at atmospheric pressure. The atypical sample A has similar temperature dependence as sample B, but the density is lower by about 0.3−0.4%. The measurements for sample B[25] were made in a commercial vibrating tube densimeter, whereas the measurements for sample A[8] were made in a single-sinker apparatus. Both sets of measurements have an estimated uncertainty of 0.1%. The deviations between the samples exceed the level of uncertainty in the measurements. The two models also show differences in density between the two samples.

Figure 4 shows comparisons of the two models with experimental thermal conductivity data for each sample
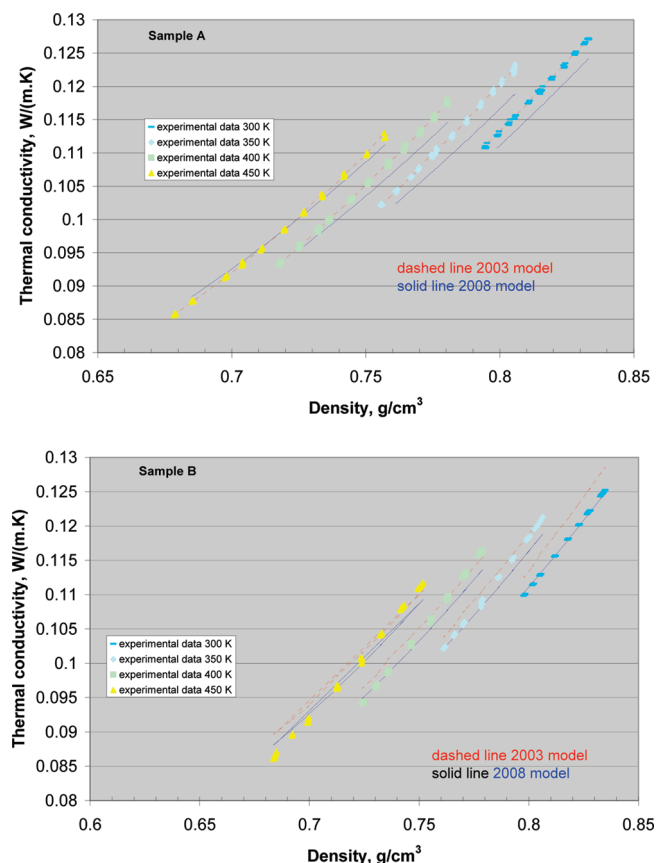
Figure 4. Thermal conductivity of RP-1, samples A and B, along with the results from both of the surrogate models.

Figure 5. Density of RP-1, samples A and B, along with the results from both of the surrogate models.

Figure 6. Distillation curves for RP-1, samples A and B, along with the results from the respective surrogate model.

(A and B) over a wide range of T and p conditions. Both sets of measurements[8,26,27] were made with the same instrument, a transient hot-wire apparatus operated at pressures up to ~70 MPa. The estimated uncertainties[8] of the measurements range from 0.5% at lower temperatures from 300 to 450 K, where decomposition and thermal radiation were not significant to approximately 1% at 550 K. The models have larger estimated uncertainties than the data, on the order of 3−4%. It is difficult to compare the data directly because they are not at exactly the same conditions of temperature and density. Therefore, we show how each model compares with the experimental data. The top panel of Figure 4 shows the thermal conductivity calculated for each model and the measurements made on sample A, and the bottom panel of Figure 4 shows the calculations and the data for sample B. Due to the large uncertainties associated with the models, it is difficult to draw conclusions beyond stating that the two samples have thermal conductivities that differ by more than their experimental uncertainties, and sample B tends to have lower thermal conductivity than that of sample A.

Figure 5 shows comparisons of the two models with experimental density data for each sample (A and B) over a wide range of T and p conditions at pressures up to 40 MPa (sample B) and 60 MPa (sample A). The density measurements on sample A were made[28] with a constant-volume technique; the
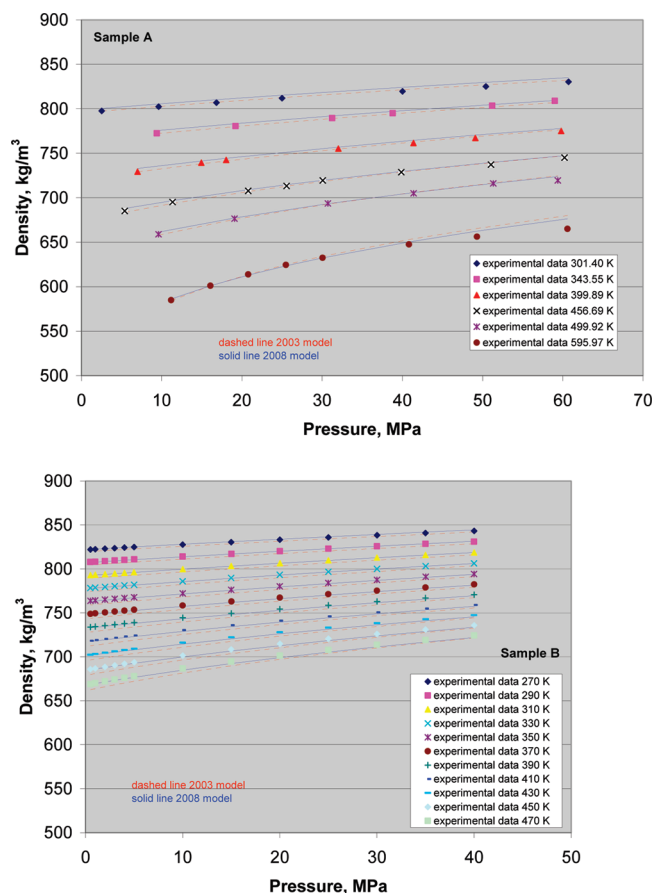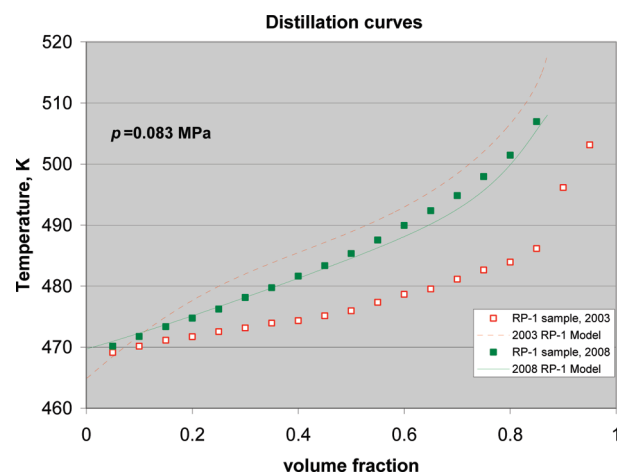
measurements on sample B with made with a different apparatus[25] that employs a vibrating tube method. Both sets of measurements have an estimated uncertainty of 0.1%. The models have larger estimated uncertainties than the data, on the order of about a half a percent. Similar to the case with the thermal conductivity data, is difficult to compare the data directly because they are not at exactly the same conditions of temperature and pressure, so we show how each model compares with the experimental data. The top panel of Figure 5 shows the density calculated for each model and

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the measurements made on sample A, and the bottom panel of Figure 5 shows the calculations and the data for sample B. Consistent with the results shown in Figure 3 (that were limited to atmospheric pressure), the density of sample A is lower than that of sample B.

Figure 6 gives the distillation curves of the two samples of RP-1. The calculated values for sample B agree very well with the experimental data. The model for the atypical sample A does not represent the shape of the distillation curve very well. It is systematically higher than the experimental data for that sample, with deviations increasing as the volume fraction increases. These deviations reach 20 K at a volume fraction of 0.85. This is due to the fact that the distillation curve was not used in the development of the model and confirms our earlier findings[21] that the distillation curve is very sensitive to sample composition. Moreover, it is clear that one can use a thermodynamic property model to represent the density and other properties well and still fail to represent the volatility behavior. The distillation curve is therefore one of the most important indicators of compositional variability of the fuel samples.

We emphasize that in the discussion above, the distillation curve that is used must consist of temperature−volume pairs that are true thermodynamic state points. For this reason, a comparison with classical distillation curve measurements is not possible. Only the results of the recently developed advanced distillation curve can be used to develop the thermodynamic model, and then be compared with that model.

Conclusions

In this paper, we have examined the variation in two thermodynamic and transport property models that were based on two different samples of the rocket kerosene, RP-1. These two samples were known to have major compositional differences. We compared model calculations of the major thermophysical properties and found that the compositional difference leads to a significant difference in the values generated by the two models. The differences between the calculated and experimental viscosities, and the calculated and experimental distillation curves are very large. The difference observed in the distillation curves are especially striking. This demonstrated sensitivity of the distillation curve to compositional variations, and we conclude that this technique is especially important in assessing such variations. We further conclude that a comprehensive study of the actual compositional variability of RP-1 is necessary.