Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Direct Sugar to Hydrocarbon Diesel (DSH-76) and Binary Mixtures of N-Hexadecane and 2,2,4,6,6-Pentamethylheptane

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S Supporting Information

ABSTRACT: The physical properties of direct sugar to hydrocarbon diesel (DSH-76) and several binary mixtures of n-hexadecane and 2,2,4,6,6-pentamethylheptane were measured in this work. The density and viscosity were measured at temperatures ranging from (293.15 to 393.15) K, and the pure component values fell within the range of previously reported values. Speed of sound data at temperatures ranging from (293.15 to 323.15) K increased from (1089 to 1357) m·s^{-1}. The bulk modulus was calculated from the density and speed of sound data, and its values ranged from (858 to 1425) MPa. Flash point values ranged from (318 to 408) K, and the surface tension values ranged from (21.8 to 27.3) mN·m^{-1}. The values of density, viscosity, speed of sound, bulk modulus, flash point (378 K), and surface tension (25.0 mN·m^{-1}) for the DSH-76 fell within the range of values measured for the binary mixtures of n-hexadecane and 2,2,4,6,6-pentamethylheptane. These data suggest that a binary mixture of n-hexadecane and 2,2,4,6,6-pentamethylheptane may be a suitable surrogate for renewable fuels such as DSH-76.
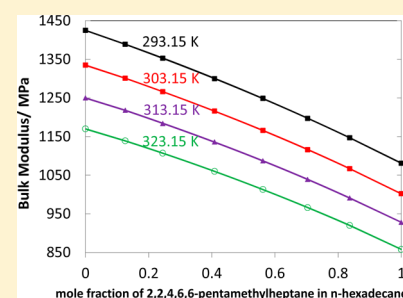
1. INTRODUCTION

Industrialized nations are developing and testing alternative fuels from abundant and renewable natural resources including plant sources, such as camelina, sugar, and algae, as well as agricultural byproducts such as tallow. As part of the development and testing process, numerical modeling of the fuel's combustion is being employed. Combustion modeling can be greatly simplified if a surrogate mixture, containing few components with well-defined physical and chemical properties, can be found that closely approximate critical fuel properties.[1] Previous researchers have used various combinations of aromatic hydrocarbons, cycloalkanes, n-alkanes, and branched alkanes to develop surrogate mixtures for petroleum-based fuels such rocket propellants, aviation fuels, coal-derived liquid fuel, petroleum diesel fuel, and for alternative fuels such as biodiesel, camelina and tallow-based hydrotreated renewable jet fuel, and algal-based hydrotreated renewable diesel fuel (algal HRD-76).[2−19] For algal HRD-76, surrogate mixtures have contained one or more linear alkanes, including n-pentadecane, n-hexadecane, n-heptadecane, and n-octadecane, and branched alkanes, including 2-methyloctane, 2-methylnonane, 2,2,4-trimethylpentane (isooctane), 2,2,4,4,6,8,8-heptamethylnonane (isocetane), and a mixture of isododecane isomers.[2−5] Several surrogates containing linear alkanes and a mixture of isododecane isomers have approximated the combustion metrics of algal HRD-76 when burned in diesel engines.[3,5] In this work, the physical properties of new surrogate mixtures

containing n-hexadecane and one isomer of isododecane, 2,2,4,6,6-pentamethylheptane, were measured and compared with algal HRD-76 and a new alternative fuel derived from sugar, direct sugar to hydrocarbon fuel (DSH-76).

In the development of a surrogate mixture, the physical properties that are important to the delivery of the fuel and the combustion process are measured. Some commonly measured properties include density, viscosity, speed of sound, and distillation curve.[2,6,8,11,13] Viscosity, surface tension, and density are also among the parameters needed by modelers to simulate the vaporization of multicomponent droplets.[20] From density and speed of sound measurements, the bulk modulus can be calculated, which impacts fuel injection time.[2,21] Other properties, such as the flash point, are part of the specifications for military diesel fuel.[22] Previous studies have measured the density, viscosity, speed of sound, surface tension, and flash point of one set of binary mixtures that could be used as surrogate for algal HRD-76,[4] n-hexadecane, and 2,2,4,4,6,8,8-heptanemethylnonane. In this work, these same properties are measured for binary mixtures of n-hexadecane and 2,2,4,6,6-pentamethylheptane.

2. MATERIALS

The *n*-hexadecane and 2,2,4,6,6-pentamethylheptane were used as received from the supplier (Table 1). Mixtures of *n*-

Table 1. Sample Information

chemical name	source	mole fraction purity	analysis method
n-hexadecane	Aldrich	>0.99	GC[a]
2,2,4,6,6-pentamethylheptane	TCI	>0.98	GC[a]

[a]Gas−liquid chromatography.

hexadecane and 2,2,4,6,6-pentamethylheptane were prepared at 293.15 K by weighing each component on a Mettler Toledo AG204 analytical balance with an error of 0.0005 g. The error in mole fraction of 2,2,4,6,6-pentamethylheptane as given by the combined expanded uncertainty is 0.0001. The sugar-based diesel fuel (DSH-76) was provided by Naval Fuels and Lubricants Cross Function Team at Patuxent River, Maryland (PAX River). The DSH-76 was produced by Amyris, which uses proprietary yeast to generate a mixture of farnesene isomers that are hydrogenated and further processed to form diesel fuel.

3. METHODS

An SVM 3000 Stabinger viscometer (Anton Paar) was used to measure the density and viscosity of the DSH-76, the organic liquids, and their mixtures, while a DSA 5000 density and sound analyzer (Anton Paar) was used to measure the speed of sound and also density. The methods for determining accuracy for these instruments using external standards are given in Luning Prak et al.[23] Duplicate or triplicate samples of each individual liquid or liquid mixture were measured at nine temperatures between (293.15 and 373.15) K using the SVM 3000, and these replicate measurements were used to determine the precision of the measurement. Duplicate samples of each individual liquid or liquid mixture were measured at four temperatures between (293.15 and 323.15) K for the DSA 5000, and these replicates were used to determine the precision of the measurement. The uncertainties in density, viscosity, and speed of sound were calculated as combined expanded uncertainties, which are the standard deviations of the measurements, multiplied by 2. The coverage factor of 2 yields a 95 % confidence interval.

A Kruss DS100 axisymmetric drop shape analyzer was used to measure the surface tension of the DSH-76, the organic liquids, and their mixtures. In the DS100, a droplet of the organic phase is formed in air. The system takes an image of the droplet, enlarges it, and analyzes the droplet shape by fitting it with the Young−LaPlace equation using the densities of the air and the organic phase.[24,25] Over 15 measurements were taken for three droplets of each liquid as has been done in previous studies.[2,4]

The flash points of the DSH-76, the organic liquids, and their mixtures were measured using a Setaflash Series 8 closed cup flash point tester model 82000-0 (Stanhope-Seta) using temperature ramping setting. This flash point model conforms to ASTM D3828 (gas ignition option), ASTM D1655 (gas ignition option), ASTM D3278, ASTM D7236, and ASTM E502 as described in the manufacturer's literature. The flashpoint of *n*-decane (Aldrich, > 99 % pure) was measured to be 322 ± 1 K, which matches the closed-cup literature value of 321 K.[26]

The DSH-76 fuel composition was characterized by gas chromatography−mass spectrometry (GC-MS) using methods described in Begue et al.[27] GC-MS data were acquired with an Agilent 7890 GC equipped with an Agilent 5975C mass selective detector configured for electron impact ionization. Samples were diluted to 1:100 in dichloromethane, and injections of 1.0 μL were made with an autoinjector. An AT-1 cross-linked methylsiloxane capillary column (50 m × 0.25 mm ID, 0.20 μm film thickness) was used with an oven temperature program that initiated data collection at a temperature of 40 °C and ramped at 10 °C·min⁻¹ to 290 °C, holding this temperature for the remaining duration of the data collection. Data were collected over column retention times from (5.1 to 36.5) min at a frequency of about 2.6 mass spectra per second, and *m/z* ratios spanning 40 to 350 mass units. Compound assignments were made using the NIST/EPA/NIH Mass Spectral Library v.2.0g, and compound abundances were estimated from normalized peak areas.

4. RESULTS

4.1. Fuel Composition. The composition of this DSH-76 alternative fuel was found to be composed entirely of alkanes and isoalkanes. The major component was 2,6,10-trimethyl dodecane (Farnesane) (92.7 mass %). Trace amounts (in mass percent) of heptadecane (3.4 %), hexadecane (2.7 %), and heptane (1.2 %) were identified as well.

Table 2. Experimental Values of Density ρ (kg·m⁻³) of DSH-76 and Mixtures of 2,2,4,6,6-Pentamethylheptane (1) in *n*-Hexadecane (2) from T = (293 to 373) K at 0.1 MPa[a]

		x_1							
T/K	DSH-76	0.000	0.1261	0.2449	0.4087	0.5620	0.7036	0.8368	1.0000
293.15	769.8	773.7	770.6	767.8	763.6	759.5	755.3	751.0	745.5
303.15	762.8	766.8	763.8	760.9	756.8	752.6	748.3	743.9	738.2
313.15	755.7	759.9	756.8	754.0	749.8	745.6	741.3	736.8	730.9
323.15	748.5	752.9	749.9	747.1	742.9	738.6	734.2	729.6	723.5
333.15	741.4	746.0	742.9	740.1	735.8	731.5	727.0	722.3	716.1
343.15	734.2	739.0	735.9	733.0	728.7	724.4	719.7	714.9	708.6
353.15	727.0	731.9	728.8	725.9	721.5	717.1	712.3	707.5	700.9
363.15	719.7	724.8	721.7	718.8	714.4	709.8	704.9	700.0	693.2
373.15	712.8	717.7	714.5	711.7	707.1	702.5	697.5	692.3	685.5

[a]x_1 is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + *n*-hexadecane) mixture. Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainties U_c are $U(x_1)$ = 0.0001 and $U_c(\rho)$ = 0.2 kg·m⁻³ (level of confidence = 0.95, $k \approx 2$).

4.2. Density. The density values of 2,2,4,6,6-pentamethyl-heptane, n-hexadecane, and their mixtures are given in Table 2 as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1). Additionally the density of 2,2,4,6,6-pentamethyl-heptane was measured to be 752.5 kg·m^{-3} at 283.15 K. The density values from the DSA 5000 and the SVM 3000 agreed with each other.

The densities of n-hexadecane of (773.7 ± 0.2, 766.8 ± 0.2, 759.9 ± 0.2, 752.9 ± 0.2, 746.0 ± 0.2, 731.9 ± 0.2, and 717.7 ± 0.2) kg·m^{-3} at (293.15, 303.15, 313.15, 323.15, 333.15, 353.15, and 373.15) K, respectively, agree with (773.6 ± 0.3, 766.7 ± 0.2, 759.7 ± 0.3, 752.9 ± 0.2, 745.8 ± 0.3, 731.8 ± 0.3, and 718.0 ± 0.3) kg·m^{-3}, measured using the same apparatus at the same temperatures.[4] The measured density of 2,2,4,6,6-pentamethylheptane of 745.5 ± 0.2 kg·m^{-3} at 293.15 K is within the range of previously reported values that are summarized by Marsh:[28] (745.0 ± 0.60, 746.3 ± 1.00, and 748.6 ± 1.00) kg·m^{-3}. At 313.15 K, Suri[29] reported a density of 731.5 ± 0.4 kg·m^{-3}, which matches the value measured herein of 730.9 ± 0.2 kg·m^{-3} within the level of measurement uncertainty. A value in the data summary by Marsh[28] at 328.15 K is slightly higher than would be predicted by the data found herein as shown in Figure 1 with other literature values.
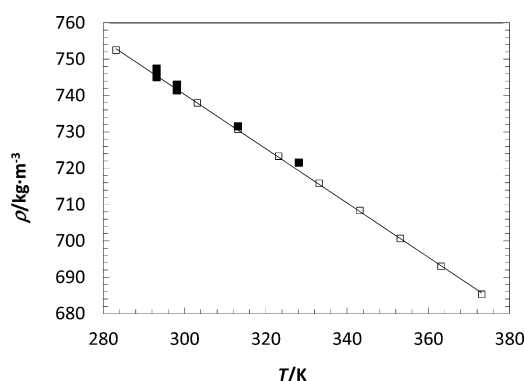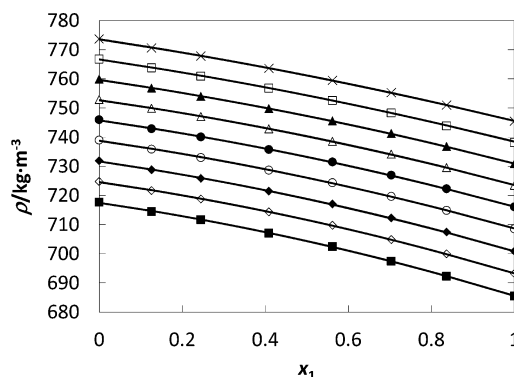

Figure 1. Density of 2,2,4,6,6-pentamethyl heptane: □, this study; ■, ref 28. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$), are smaller than the symbols.

For the mixtures, the density decreased as the mole fraction of 2,2,4,6,6-pentamethylheptane increased, but the decrease was not linear as shown in Figure 2. Density and mole fraction data were fit to a second-order polynomial:

$$\rho / \text{kg·m}^{-3} = A x_1^2 + B x_1 + C \tag{1}$$

In this equation x_1 is the mole fraction of 2,2,4,6,6-pentamethylheptane, and A, B, and C are fitting parameters, which are given in Table 3. Microsoft Excel 2010 was used to fit the polynomial to the data, and the standard deviation of the fit (Table 3) was calculated by multiplying the standard error of the fit by the square root of the number of data points. The fits are good with $R^2 > 0.999$.

A deviation from a linear relationship between density and mole fraction suggests that the mixtures are nonideal solutions. Deviations from ideal behavior can be quantified by examining the excess molar volume and excess density. Fermeglia and Torriano[30] showed that excess molar volumes (V_m^E) of mixtures of n-hexadecane with branched alkanes had their greatest deviation from ideal behavior at mole fractions close to 0.5. An ideal solution would have an excess molar volume equal

Figure 2. Density of (2,2,4,6,6 pentamethylheptane (x_1) + n-hexadecane) mixtures at ×, 293.15 K; □, 303.15 K; ▲, 313.15 K; △, 323.15 K; ●, 333.15 K; ○, 343.15 K; ◆, 353.15 K; ◇, 363.15 K; ■, 373.15 K, this study. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$), are smaller than the symbols. Lines shown are second order fits using eq 1 with the coefficients in Table 3.

to zero. The excess molar volumes of two-component mixtures of n-hexadecane with isooctane (iC-8), 2,2,4,4,6,8,8-heptame-thylnonane (iC-16), 2,6,10,14-tetramethylpentadecane (iC-19), and 2,6,10,15,19,23-tetracosane (iC-30) were (−0.496, 0.126, 0.109, and 0.064) cm^3·mol^{-1}, respectively, at mole fractions close to 0.5 and 293 K.[30] Steiger et al.[31] also found negative excess molar volumes of mixtures of n-hexadecane with branched alkanes at a mole fraction equal to 0.5. At 293 K, their two-component mixtures of n-hexadecane with branched heptanes had excess molar volumes that ranged from (−0.198 to −0.545) cm^3·mol^{-1}, which exhibit a greater deviation from an ideal liquid than those of mixtures of n-hexadecane with branched octanes (−0.133 to −0.233) cm^3·mol^{-1} and those of mixtures of n-hexadecane with branched decanes (−0.035 to −0.077) cm^3·mol^{-1}.[31] In the current study, the excess molar volumes (V_m^E) for the 0.5620 mole fraction of 2,2,4,6,6-pentamethylheptane in n-hexadecane were calculated using

$$V_m^E = \frac{M_1 x_1 + M_2 x_2}{\rho_m} - \frac{M_1 x_1}{\rho_1} - \frac{M_2 x_2}{\rho_2} \tag{2}$$

where ρ_m is the density of the mixture, ρ_1 and ρ_2 are the densities, M_1 and M_2 are the molar masses, and x_1 and x_2 are the mole fractions of 2,2,4,6,6-pentamethylheptane as component 1 and n-hexadecane as component 2. The excess molar volumes for the 0.5620 mole fraction of 2,2,4,6,6-pentam-ethylheptane in n-hexadecane at each temperature are given in Table 3. At 293.15 K, the excess molar volume of 0.03 cm^3·mol^{-1} is small and falls between the excess molar volumes found for n-hexadecane with a branched hexadecane (0.126 cm^3·mol^{-1}) and with various branched decanes (−0.035 to −0.077 cm^3·mol^{-1}).[30,31] At 303.15 K, the excess molar volume is negative, −0.04 cm^3 mol^{-1}, and deviates more from an ideal solution as temperature increases. The greater deviation from an ideal solution with increasing temperature has also been found for mixtures of n-hexadecane with various branched heptanes[31] and for mixtures of decalin with linear alkanes from nonane to undecane.[32]

The excess density also shows the deviation of a real solution from an ideal mixture. The excess density was calculated from

$$\rho^E = \rho_m - (x_1 \rho_1) - (x_2 \rho_2) \tag{3}$$

Table 3. Parameters for Equation 1, $\rho/\text{kg}\cdot\text{m}^{-3} = Ax_1^2 + Bx_1 + C$, Which Correlates Density ρ ($\text{kg}\cdot\text{m}^{-3}$) to Mole Fraction of 2,2,4,6,6-Pentamethylheptane (x_1) in n-Hexadecane, and the Excess Molar Volume (V_m^E) and Excess Density (ρ^E) at x_1 = 0.5620, T = (293 to 373) K, and 0.1 MPa[a]

T/K	A	B	C	R^2	standard deviation of fit	V_m^E $\text{cm}^3\cdot\text{mol}^{-1}$	ρ^E $\text{kg}\cdot\text{m}^{-3}$
293.15	-6.4 ± 1.2	-21.6 ± 1.2	773.6 ± 0.3	0.9999	0.344	0.03	1.6
303.15	-7.3 ± 1.2	-21.1 ± 1.2	766.7 ± 0.3	0.9999	0.350	-0.04	1.9
313.15	-7.8 ± 1.6	-20.9 ± 1.6	759.7 ± 0.3	0.9998	0.449	-0.08	2.0
323.15	-8.8 ± 1.6	-20.3 ± 1.6	752.7 ± 0.3	0.9999	0.395	-0.15	2.2
333.15	-9.0 ± 1.6	-20.6 ± 1.6	745.8 ± 0.3	0.9998	0.461	-0.18	2.3
343.15	-9.5 ± 1.7	-20.6 ± 1.8	738.8 ± 0.4	0.9998	0.500	-0.24	2.5
353.15	-10.1 ± 1.7	-20.7 ± 1.7	731.7 ± 0.4	0.9997	0.488	-0.29	2.6
363.15	-10.8 ± 1.5	-20.5 ± 1.6	724.6 ± 0.4	0.9999	0.442	-0.34	2.8
373.15	-11.3 ± 1.7	-20.6 ± 1.7	717.5 ± 0.4	0.9998	0.479	-0.39	2.9

[a]The error represents the 95 % confidence interval.

where ρ_m is the density of the binary mixture, ρ_1 and ρ_2 are the densities of the pure components, and x_1 and x_2 are the mole fractions of 2,2,4,6,6-pentamethylheptane as component 1 and n-hexadecane as component 2. The calculated values of excess density for 0.5620 mole fraction of 2,2,4,6,6-pentamethylheptane in n-hexadecane are given in Table 3, with all of the remaining mixtures given in Table S1 of the Supporting Information. Figure 3 shows that the excess density values for
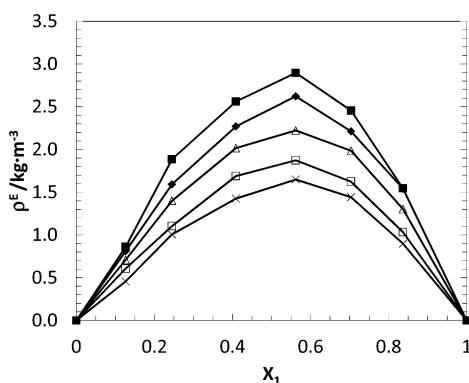
Figure 3. Excess density of (2,2,4,6,6 pentamethylheptane (x_1) + n-hexadecane) mixtures at select temperatures as calculated by eq 6: at ×, 293.15 K; □, 303.15 K; △, 323.15 K; ◆, 353.15 K; ■, 373.15 K.

all solutions show a positive deviation from ideal behavior. These results suggest that the molecules are more closely packed together than would be predicted from their individual densities. At 373.15 K, the excess density for 0.5620 mole fraction of 2,2,4,6,6-pentamethylheptane in n-hexadecane is 2.9 $\text{kg}\cdot\text{m}^{-3}$, which is only 2.8 % of the density value of 702.5 $\text{kg}\cdot\text{m}^{-3}$ at this temperature and mole fraction.

The density values for the DSH-76 are also given in Table 2. The DSH-76 density values fall within the values measured for the 2,2,4,6,6-pentamethylheptane and hexadecane mixtures. When comparing to other alternative fuels, the density of hydroprocessed renewable jet fuel (HRJ) from camelina and tallow with density values at 293.15 K of (764.4 and 753.6) $\text{kg}\cdot\text{m}^{-3}$, respectively, also fall within this density range, but the density of algal-based hydrotreated renewable diesel fuel with a density of 776.1 $\pm$ 1.3 $\text{kg}\cdot\text{m}^{-3}$ is higher than the density range of the mixtures measured herein.[4,23]

4.3. Viscosity. The dynamic and kinematic viscosity values for n-hexadecane, 2,2,4,6,6-pentamethylheptane, and their

mixtures are given in Table 4 as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1). The viscosities of n-hexadecane of (3.44, 2.21, 1.53, 1.13, and 0.876) mPa·s at (293.15, 313.15, 333.15, 353.15, and 373.15) K, respectively agree with (3.46 $\pm$ 0.04, 2.23 $\pm$ 0.04, 1.55 $\pm$ 0.04, 1.14 $\pm$ 0.04, and 0.886 $\pm$ 0.04) mPa·s, measured using the same apparatus.[4] For 2,2,4,6,6-pentamethylheptane, the viscosity values reported by Sanin and Melenteva[33] are shown in Figure 4 along with data reported herein. The value of 0.827 $\pm$ 0.005 mPa·s at 323.15 K agrees with 0.825 mPa·s from Sanin and Melenteva.[33]

Kinematic viscosity data were fit to the McAllister three-body model:[34]

$$\ln \nu_m = x_1^3 \ln \nu_1 + 3x_1^2 x_2 \ln \nu_{1,2} + 3x_1 x_2^2 \ln \nu_{2,1} + x_2^3 \ln \nu_2$$
$$- \ln\left(x_1 + x_2 \frac{M_2}{M_1}\right) + 3x_1^2 x_2 \ln\left(\frac{1}{3}\left(2 + \frac{M_2}{M_1}\right)\right)$$
$$+ 3x_1 x_2^2 \ln\left(\frac{1}{3}\left(1 + 2\frac{M_2}{M_1}\right)\right) + x_2^3 \ln\left(\frac{M_2}{M_1}\right) \quad (4)$$

where ν_m is the kinematic viscosity of the binary mixture, ν_1 and ν_2 are the kinematic viscosities of the pure components, M_1 and M_2 are the molar masses, and x_1 and x_2 are the mole fractions of 2,2,4,6,6-pentamethylheptane as component 1 and n-hexadecane as component 2. The interaction parameters $\nu_{2,1}$ and $\nu_{1,2}$ were determined using the GRG nonlinear engine of the SOLVER function in Microsoft Excel 2010 to minimize the sum of the square of the difference between the model and the measured kinematic viscosity:

$$\min \sum (\text{model} - \text{experimental data})^2 \quad (5)$$

The standard deviation for the fit (σ) was determined by

$$\sigma = \sqrt{\frac{\sum (\nu_m - \nu_{m,cal})^2}{N - n}} \quad (6)$$

where ν_m is the kinematic viscosity of the binary mixture, $\nu_{m,calc}$ is the value calculated by eq 4, N is the number of experimental data, and n is the number of parameters in the fitting equation. The values of $\nu_{2,1}$, $\nu_{1,2}$, and σ are given in Table 5 for each temperature. Figure 5 shows that the model fits the data well.

The excess viscosity ($\Delta\nu$) of each mixture was calculated using:

$$\nu^E = \nu_m - (x_1\nu_1) - (x_2\nu_2) \quad (7)$$

Table 4. Experimental Values of Dynamic Viscosity η (mPa·s) and Kinematic Viscosity ν (mm^2·s^{-1}) for DSH-76 and the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) from T = (293 to 373) K at 0.1 MPa^a

			x_1							
T/K		DSH-76	0.000	0.1261	0.2449	0.4087	0.5620	0.7036	0.8368	1.0000
293.15	η/mPa·s	2.74	3.44	3.10	2.79	2.41	2.09	1.80	1.56	1.29
	ν/mm^2·s^{-1}	3.56	4.44	4.02	3.64	3.16	2.75	2.38	2.07	1.74
303.15	η/mPa·s	2.16	2.72	2.47	2.25	1.97	1.72	1.50	1.31	1.10
	ν/mm^2·s^{-1}	2.83	3.55	3.24	2.96	2.60	2.29	2.00	1.76	1.49
313.15	η/mPa·s	1.76	2.21	2.03	1.86	1.64	1.44	1.27	1.11	0.94(1)
	ν/mm^2·s^{-1}	2.32	2.91	2.68	2.46	2.18	1.94	1.71	1.51	1.29
323.15	η/mPa·s	1.45	1.82	1.68	1.55	1.38	1.23	1.09	0.96(6)	0.82(7)
	ν/mm^2·s^{-1}	1.94	2.42	2.24	2.07	1.86	1.66	1.48	1.32	1.14
333.15	η/mPa·s	1.22	1.53	1.42	1.32	1.18	1.06	0.94(4)	0.84(3)	0.72(6)
	ν/mm^2·s^{-1}	1.65	2.06	1.91	1.78	1.60	1.45	1.30	1.17	1.01
343.15	η/mPa·s	1.05	1.31	1.22	1.14	1.02	0.922	0.827	0.742	0.643
	ν/mm^2·s^{-1}	1.42	1.77	1.66	1.55	1.40	1.27	1.15	1.04	0.90(8)
353.15	η/mPa·s	0.90(7)	1.13	1.06	0.98(8)	0.89(4)	0.81(0)	0.73(0)	0.65(8)	0.57(3)
	ν/mm^2·s^{-1}	1.25	1.55	1.45	1.36	1.24	1.13	1.03	0.93(0)	0.81(8)
363.15	η/mPa·s	0.79(6)	0.99(0)	0.92(8)	0.87(0)	0.79(1)	0.71(9)	0.65(1)	0.58(9)	0.51(5)
	ν/mm^2·s^{-1}	1.10	1.37	1.29	1.21	1.11	1.01	0.92(3)	0.84(1)	0.74(3)
373.15	η/mPa·s	0.70(6)	0.87(6)	0.82(3)	0.77(3)	0.70(6)	0.64(4)	0.58(5)	0.53(1)	0.46(7)
	ν/mm^2·s^{-1}	0.99(0)	1.22	1.15	1.09	1.00	0.91(7)	0.83(9)	0.76(7)	0.68(1)

$^a x_1$ is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + n-hexadecane) mixture. Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainties U_c are $U(x_1)$ = 0.0001, $U_c(\eta)$ = 0.01 mPa·s, and $U_c(\nu)$ = 0.01 mm^2·s^{-1} (level of confidence = 0.95, $k \approx 2$).
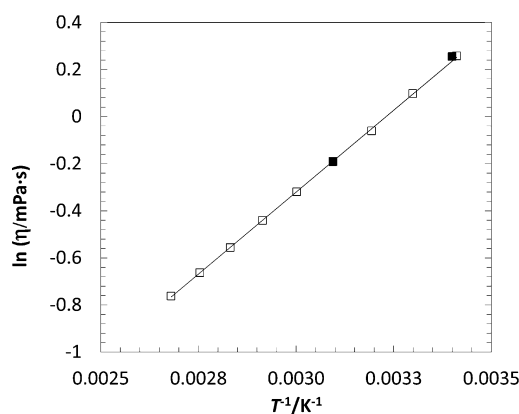

Figure 4. Viscosity of 2,2,4,6,6-pentamethylheptane: □, this study; ■, ref 33. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$), are smaller than the symbols.
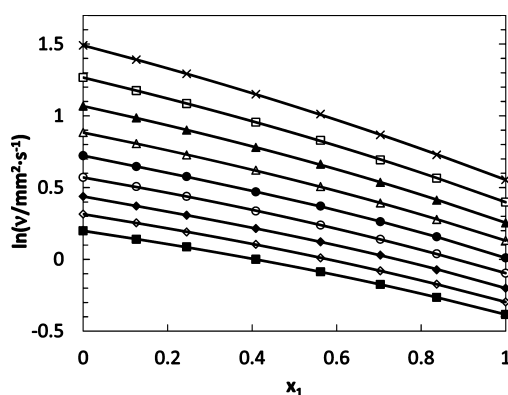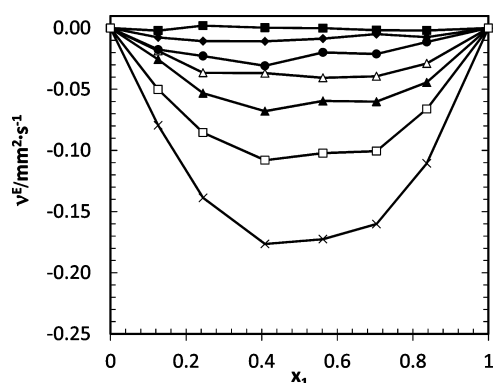

Figure 5. Viscosity of (2,2,4,6,6 pentamethylheptane (x_1) + n-hexadecane) mixtures: at ×, 293.15 K; □, 303.15 K; ▲, 313.15 K; △, 323.15 K; ●, 333.15 K; O, 343.15 K; ◆, 353.15 K; ◇, 363.15 K; ■, 373.15 K. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$), are smaller than the symbols. Lines shown are fits to eq 4 with the coefficients in Table 5.

Table 5. Values of the Coefficients for McAllister Equation (eq 4) and Associated Standard Deviations (eq 6) for Mixtures of the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) from T = (293 to 373) K at 0.1 MPa

T/K	ν_{12} mm^2·s^{-1}	ν_{21} mm^2·s^{-1}	σ mm^2·s^{-1}
293.15	2.54	3.45	0.0073
303.15	2.14	2.81	0.0058
313.15	1.83	2.35	0.0051
323.15	1.58	1.99	0.0038
333.15	1.40	1.69	0.0029
343.15	1.21	1.50	0.0026
353.15	1.09	1.31	0.0017
363.15	0.97	1.17	0.0016
373.15	0.89	1.06	0.0014

where ν_m is the kinematic viscosity of the binary mixture, ν_1 and ν_2 are the kinematic viscosities of the pure components, and x_1 and x_2 are the mole fractions of 2,2,4,6,6-pentamethylheptane as component 1 and n-hexadecane as component 2. The calculated values of the excess viscosity are given in Table S2 of the Supporting Information. Figure 6 shows that the viscosity deviations are small and negative and that the deviations approach zero as temperature increases. This negative deviation from ideal behavior suggest that the molecules slide past each other more easily in solution than would be predicted from their individual viscosities. At 293.15 K, the excess viscosity for 0.5620 mole fraction of 2,2,4,6,6-pentamethylheptane in n-hexadecane is 0.17 mm^2·s^{-1}, which is only 6 % of the viscosity value of 2.75 mm^2·s^{-1} at this temperature and mole fraction.

Figure 6. Excess viscosity of (2,2,4,6,6-pentamethylheptane (x_1) + n-hexadecane) mixtures at select temperatures as calculated by eq 7: at ×, 293.15 K; □, 303.15 K; ▲, 313.15 K; △, 323.15 K; ●, 333.15 K; ◆, 353.15 K; ■, 373.15 K.

The viscosity values of the DSH-76 at various temperature are also given in Table 4. The viscosity of the DSH-76 falls within the values measured for the 2,2,4,6,6-pentamethylheptane and hexadecane mixtures. When comparing to other alternative fuels at 293.15 K, the viscosity values of (1.97, 1.41, and 3.40) mPa·s for HRJ from camelina, HRJ from tallow, and algal-based hydrotreated renewable diesel fuel, respectively, also fall within the viscosity values of the mixtures measured herein, (1.29 to 3.44) mPa·s.[4,23]

4.4. Speed of Sound and Bulk Modulus. The speed of sound for the n-hexadecane, 2,2,4,6,6-pentamethylheptane, and their mixtures are given in Table 6 as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1). The values for n-hexadecane come from Luning Prak et al.[4] The speed of sound decreases as the percentage of 2,2,4,6,6-pentamethylheptane in the mixture increases (Table 6). The speed of sound decreases with increasing temperature (Table 6) and is linear over the temperature range studied. Speed of sound and temperature data were fit to

$$c/\mathrm{m\cdot s^{-1}} = AT/\mathrm{K} + B \qquad (8)$$

using the Microsoft Excel linear regression software in its Analysis Toolpak, and the standard deviation of the fit was calculated by multiplying the standard error of the fit by the square root of the number of data points. The fitting parameters are given in Table 7, and all fits are good with an $R^2 > 0.9999$. These lines are shown in Figure 7.

The isentropic bulk modulus, E_v, was calculated at each temperature and ambient pressure from the speed of sound (c) and density (ρ) by:[35]

Table 7. Parameters for Equation 8: $c = AT/K + B$, Which Relates Speed of Sound, c ($m\cdot s^{-1}$), to Temperature for $T = (293\ \text{to}\ 323)\ K^a$ for DSH-76 and the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) at 0.1 MPa

x_1	$A/\mathrm{K^{-1}}$	$B/\mathrm{m\cdot s^{-1}}$	R^2	standard deviation of fit
0.1261	−3.67 ± 0.11	2419 ± 34	0.9999	1.13
0.2449	−3.67 ± 0.09	2404 ± 34	0.9999	0.920
0.4087	−3.68 ± 0.10	2382 ± 34	0.9999	0.992
0.5620	−3.70 ± 0.10	2367 ± 29	0.9999	0.990
0.7036	−3.73 ± 0.10	2352 ± 29	0.9999	0.990
0.8368	−3.76 ± 0.10	2339 ± 31	0.9999	1.06
1.000	−3.82 ± 0.12	2324 ± 36	0.9999	1.20
DSH-76	−3.75 ± 0.11	2406 ± 34	0.9999	1.13

^{a}Error bars are the 95 % confidence interval.
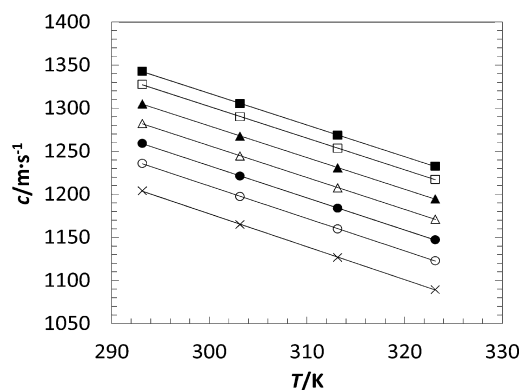
Figure 7. Speed of sound of (2,2,4,6,6-pentamethylheptane (x_1) + n-hexadecane) mixtures at various mole fractions: ■, $x_1 = 0.1261$; □, $x_1 = 0.2449$; ▲, $x_1 = 0.4089$; △, $x_1 = 0.5620$; ●, $x_1 = 0.7036$; ○, $x_1 = 0.8368$; ×, $x_1 = 1.000$. Error bars, which are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$), are smaller than the symbols. Lines shown are fits to eq 8 with the coefficients in Table 7.

$$E_v/\mathrm{Pa} = (c^2/\mathrm{m^2\cdot s^{-2}})(\rho/\mathrm{kg\cdot m^{-3}}) \qquad (9)$$

These values are given in Table 8. The n-hexadecane bulk modulus values were taken from Luning Prak et al.[4] The bulk modulus decreases as the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1) in n-hexadecane increases and as temperature increases.

The speed of sound and isentropic bulk modulus for the DSH-76 are also given in Tables 6 and 8, respectively. The speed of sound and isentropic bulk modulus of the DSH-76 fall within the values measured for 2,2,4,6,6-pentamethylheptane and hexadecane mixtures at all temperatures tested. When

Table 6. Experimental Values of Speed of Sound Measurements c ($m\cdot s^{-1}$) for DSH-76 and the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) from $T = (283\ \text{to}\ 323)\ K$ at 0.1 MPa^a

		x_1							
T/K	DSH-76	0.000	0.1261	0.2449	0.4087	0.5620	0.7036	0.8368	1.0000
293.15	1308.5	1357.0^b	1342.7	1327.4	1304.9	1282.2	1259.1	1235.8	1204.0
303.15	1270.2	1319.5^b	1305.2	1290.0	1267.4	1244.5	1221.1	1197.4	1164.9
313.15	1232.8	1282.8^b	1268.4	1253.3	1230.7	1207.5	1183.8	1159.8	1126.7
323.15	1196.1	1246.8^b	1232.5	1217.2	1194.6	1171.2	1147.2	1122.9	1089.3

$^a x_1$ is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + n-hexadecane) mixture. Standard uncertainties u are $u(T) = 0.01$ K, and combined expanded uncertainties U_c are $U(x_1) = 0.0001$ and $U_c(c) = 0.3$ m·s^{-1} (level of confidence = 0.95, $k \approx 2$). ^{b}Taken from ref 4.

Table 8. Calculated Isentropic Bulk Modulus of Mixtures E_v (MPa) for DSH-76 and the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) from T = (283 K to 323) K at 0.1 MPa[a]

		x_1							
T/K	DSH-76	0.000	0.1261	0.2449	0.4087	0.5620	0.7036	0.8368	1.0000
293.15	1317	1425[b]	1389	1353	1300	1249	1197	1147	1081
303.15	1230	1335[b]	1301	1266	1216	1166	1116	1067	1002
313.15	1148	1250[b]	1218	1184	1136	1087	1039	991	928
323.15	1070	1170[b]	1139	1107	1060	1013	966	920	858

[a]x_1 is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + n-hexadecane) mixture. Standard uncertainties u are $u(T)$ = 0.01 K, and combined expanded uncertainties U_c are $U(x_1)$ = 0.0001 and $U_c(E_v)$ = 0.4 MPa (level of confidence = 0.95, $k \approx 2$). [b]Taken from ref 4.

Table 9. Experimental Values of Flash Point and Surface Tension for DSH-76 and the System of 2,2,4,6,6-Pentamethylheptane (1) in n-Hexadecane (2) at 0.1 MPa[a]

		x_1							
	DSH-76	0.0000	0.1261	0.2449	0.4087	0.5620	0.7036	0.8368	1.0000
flash point/K	378	408[b]	360 ± 3	346	336	330	325	322	318
surface tension/mN·m^{-1}	25.0	27.3[b]	25.9 ± 0.3	25.3	24.3	23.8	23.1	22.5	21.8

[a]x_1 is the mole fraction of 2,2,4,6,6-pentamethylheptane in the (2,2,4,6,6-pentamethylheptane + n-hexadecane) mixture. Combined expanded uncertainties U_c are $U(x_1)$ = 0.0001, U_c(flash point) = 2 K, and U_c(surface tension) = 0.2 mN·m^{-1} unless indicated by the ± symbol (level of confidence = 0.95, $k \approx 2$). Surface tension measurements were taken at room temperature, 294 ± 1 K. [b]Taken from ref 4.

comparing to other alternative fuels at 293.15 K, the speed of sound values of (1301.0 ± 0.6, 1279.8 ± 0.6, and 1340.9 ± 0.6) m·s^{-1} for HRJ from camelina, HRJ from tallow, and algal-based hydrotreated renewable diesel fuel, respectively, fall within the speed of sound values of the mixtures measured herein, (1204 to 1357) m·s^{-1}.[4,23] The bulk modulus values at 293.15 K of (1294 ± 1, 1234 ± 1, and 1395 ± 2) MPa for HRJ from camelina, HRJ from tallow, and algal-based hydrotreated renewable diesel fuel, respectively, also fall within the bulk modulus values of the mixtures measured herein, (1081 to 1425) MPa.[4,23]

4.5. Flash Point and Surface Tension. The surface tension and flash point values for the n-hexadecane, 2,2,4,6,6-pentamethylheptane, and their mixtures are given in Table 9 as a function of the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1). The surface tension and flash point values of n-hexadecane were taken from Luning Prak et al.[4] since they were measured using the same apparati as were used to analyze the alkanes reported herein and they agreed with other literature values. No literature values were available for the surface tension or flash point of 2,2,4,6,6-pentamethylheptane. The flashpoint of 2,2,4,6,6-pentamethylheptane was estimated to be 320 K using an empirical correlation from Catorie and Naudet,[36]

$$FP/K = 1.477(T_{bp}/K)^{0.79866}(\Delta H_{vap}^o/kJ \cdot mol^{-1})^{0.16845}$$

$$n^{-0.05948} \quad\quad (10)$$

where T_{bp} is the boiling point of 451. ± 2 K,[37] $\Delta H°_{vap}$ is the standard enthalpy of vaporization of 48.97 kJ·mol^{-1},[38] and n is the number of carbon atoms in the molecule, which is 12. The authors report that the mean absolute deviation for flash points in the temperature range of (303 to 333) K was 3.5 K. The flashpoint value of 318 ± 2 K for 2,2,4,6,6-pentamethylheptane measured herein agrees with this predicted value of 320 ± 3.5 K.

For the mixtures, as the mole fraction of 2,2,4,6,6-pentamethylheptane (x_1) increases, the surface tension and flash point decrease (Figure 8), but the relationship is not linear. The flash point and surface tension of the DSH-76 are
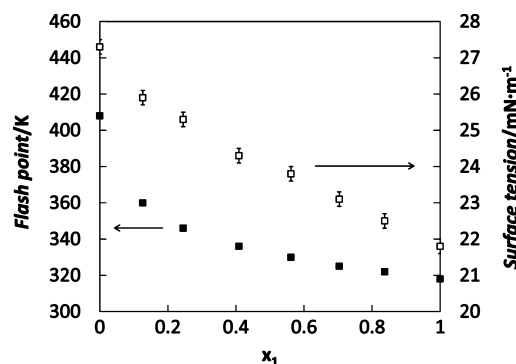
Figure 8. Flash point, ■, and surface tension, □, of (2,2,4,6,6-pentamethylheptane (x_1) + n-hexadecane) mixtures. The error bars are the combined expanded uncertainties with a 0.95 level of confidence ($k \approx 2$).

also given in Table 9. The flash point, 378 K, and surface tension, 25.0 mN·m^{-1}, of the DSH-76 fall within the values measured for the 2,2,4,6,6-pentamethylheptane and hexadecane mixtures. When comparing algal-based hydrotreated renewable diesel fuel to these mixtures, the surface tension of the algal fuel, 26.0 mN·m^{-1},[4] and the flash point, 360 K,[4] also fall within the values of the mixtures.

5. CONCLUSION

In this work, the physical properties of a two-component mixture of n-hexadecane and 2,2,4,6,6-pentamethylheptane were measured and compared with those values for a direct sugar to hydrocarbon renewable diesel fuel (DSH-76) and other hydrotreated renewable fuels. Many of the measurements of the pure components fell within values reported in the literature. A comparison of the data for DSH-76 with those of the mixtures reveals that the density, viscosity, speed of sound, bulk modulus, surface tension, and flash point fell within the range of values measured for the mixtures of n-hexadecane and 2,2,4,6,6-pentamethylheptane. Since the physical properties are similar between the DSH-76 and two-component mixtures of n-

hexadecane and 2,2,4,6,6-pentamethylheptane, one of these mixtures may serve as a reasonable surrogate in numerical modeling efforts for the combustion of DSH-76.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Values of the excess viscosity (ν^E) and excess density (ρ^E) for the mixtures of *n*-hexadecane and 2,2,4,6,6-pentamethylheptane. This material is available free of charge via the Internet at http://pubs.acs.org.

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■ REFERENCES

(1) Pitz, W. J.; Mueller, C. J. Recent progress in the development of diesel surrogate fuels. *Prog. Energy Combust. Sci.* **2011**, *37*, 340−350.

(2) Luning Prak, D. J.; Cowart, J. S.; Hamilton, L. J.; Hoang, D. T.; Brown, E. K.; Trulove, P. C. Development of a surrogate mixture for Algal-based hydrotreated renewable diesel. *Energy Fuels* **2013**, *27*, 954−961.

(3) Mathes, A.; Mathes, A. D.; Ries, J. J.; Caton, P. A.; Cowart, J. S.; Luning Prak, D.; Hamilton, L. J. Binary Mixtures of Branched and Aromatic Pure Component Fuels as Surrogates for Future Diese Fuels. *SAE Int. J. Fuel Lub.* **2010**, *3*, 794−809.

(4) Luning Prak, D. J.; Trulove, P. C.; Cowart, J. S. Density, Viscosity, Speed of Sound, Surface Tension, and Flash Point of Binary Mixtures of N-hexadecane and 2,2,4,4,6,8,8-Heptamethylnonane and of Algal-Based Hydrotreated Renewable Diesel. *J. Chem. Eng. Data* **2013**, *58*, 920−926.

(5) Hamilton, L. J.; Cowart, J. S.; Luning Prak, D. J.; Caton, P. A. An experimental study of normal-hexadecane and iso-dodecane binary fuel blends in a military diesel engine. *The Proceedings of the ASME 2012 Internal Combustion Engine Division Fall Technical Conference*, Vancouver, British Columbia, Canada, September 2012.

(6) Huber, M. L.; Lemmon, E. W.; Ott, L. S.; Bruno, T. J. Preliminary Surrogate Mixture Models for the Thermophysical Properties of Rocket Propellants RP-1 and RP-2. *Energy Fuels* **2009**, *23*, 3093−3088.

(7) Edward, T.; Maurice, L. Q. Surrogate Mixtures to Represent Complex Aviation and RocketFuels. *J. Propul. Power* **2001**, *19*, 461−466.

(8) Huber, M. L.; Lemmon, E. W.; Bruno, T. J. Surrogate mixture models for the thermophysical properties of aviation fuel Jet-A. *Energy Fuels* **2010**, *24*, 3565−3571.

(9) Wood, C. P.; McDonell, V. G.; Smith, R. A.; Samuelsen, G. S. Development and application of a surrogate distillate fuel. *J. Propul. Power* **1989**, *5*, 399−405.

(10) Bruno, T. J.; Smith, B. L. Evaluation of the physicochemical authenticity of aviation kerosene surrogate mixtures. Part 1: Analysis of volatility with the advanced distillation curve. *Energy Fuels* **2010**, *24*, 4266−4276.

(11) Bruno, T. J.; Huber, M. L. Evaluation of the physicochemical authenticity of aviation kerosene surrogate mixtures. Part 2: Analysis and prediction of thermophysical properties. *Energy Fuels* **2010**, *24*, 4277−4284.

(12) Honnet, S.; Seshadri, K.; Niemann, U.; Peters, N. A surrogate fuel for kerosene. *Proc. Combust. Inst.* **2009**, *32*, 485−492.

(13) Dooley, S.; Won, S. H.; Chaos, M.; Heyne, J.; Ju, Y. G.; Dryer, F. L.; Kumar, K.; Sung, C. J.; Wang, H. W.; Oehlschlaeger, M. A.; Santoro, R. J.; Litzinger, T. A. A jet fuel surrogate formulated by real fuel properties. *Combust. Flame* **2010**, *157*, 2343−2349.

(14) Huber, M. L.; Lemmon, E. W.; Diky, V.; Smith, B. L.; Bruno, T. J. Chemical authentic surrogate mixture model for the thermophysical properties of a coal-derived fuel. *Energy Fuels* **2008**, *22*, 3249−3257.

(15) Mueller, C. J.; Cannella, W. J.; Bruno, T. J.; Bunting, B.; Dettman, H. D.; Franz, J. A.; Huber, M. L.; Natarajan, M.; Pitz, W. J.; Ratcliff, M. A.; Wright, K. Methodology for formulating diesel surrogate fuels with accurate compositional, ignition-quality, and volatility characteristics. *Energy Fuels* **2012**, *26*, 4277−4284.

(16) Mathieu, O.; Djebaili-Chaumeix, N.; Paillard, C. E.; Douce, F. Experimental study of soot formation from a diesel fuel surrogate in a shock tube. *Combust. Flame* **2009**, *156*, 1576−1586.

(17) Lemaire, R.; Faccinetto, A.; Therssen, E.; Ziskind, M.; Focsa, C.; Desgroux, P. Experimental comparison of soot formation in turbulent flames of diesel and surrogate diesel fuels. *Proc. Combust. Inst.* **2009**, *32*, 737−744.

(18) Ramirez Lancheros, H. P.; Fikri, M.; Rincon Cancino, L.; Moreac, G.; Shulz, C.; Dagaut, P. Autoignition of surrogate biodiesel fuel (B30) at high pressure: Experimental and modeling kinetic study. *Combust. Flame* **2012**, *33*, 996−1008.

(19) Allen, C.; Valco, D.; Toulson, E.; Edwards, T.; Lee, T. Ignition behavior and surrogate modeling of JP-8 and of camelina and tallow hydrotreated renewable jet fuels at low temperature. *Combust. Flame* **2013**, *160*, 232−239.

(20) Ra, Y.; Reitz, R. D. The Application of a Multicomponent Droplet Vaporization Model to Gasoline Injection Engines. *Int. J. Engine Res.* **2003**, *4*, 193−218.

(21) Tat, M. E.; van Gerpen, J. H. *Measurement of Biodiesel Speed of Sound and Its Impacton Injection Timing*, Final Report, Report 4 in a series of 6 for National Renewable Energy Laboratory: Golden, CO, February 2003.

(22) *Performance Specification Fuel*, Naval Distillate, Military Specification MIL-PRF-16884L; Department of Defense: Washington, DC, Oct 23, 2006.

(23) Luning Prak, D. J.; Brown, E. K.; Trulove, P. C. Density, viscosity, speed of sound, and bulk modulus of methyl alkanes, dimethyl alkanes, and hydrotreated renewable fuels. *J. Chem. Eng. Data* **2013**, *58*, 2065−2075.

(24) Rotenberg, Y.; Boruvka, L.; Newmann, A. W. Determination of surface tension and contact angle from the shapes of axisymmertric fluid interfaces. *J. Colloid Interface Sci.* **1983**, *1*, 169−183.

(25) Hansen, F. K.; Rodsrud, G. Surface tension by pendant drop I. A Fast standard instrument using computer image analysis. *J. Colloid Interface Sci.* **1991**, *141*, 1−9.

(26) Affens, W. A.; Carhart, H. W.; McLaren, G. W. Variation of flammability index with temperature and the relationship to flash point of liquid hydrocarbons. *J. Fire Flamm.* **1977**, *8*, 153−159.

(27) Begue, N. J.; Cramer, J. A.; Von Bargen, C.; Myers, K. M.; Johnson, K. J.; Morris, R. E. Automated Method for Determining Hydrocarbon Distributions in Mobility Fuels. *Energy Fuels* **2011**, *25*, 1617−1623.

(28) *Densities of Aliphatic Hydrocarbons: Alkanes (Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology - New Series/Physical Chemistry)*, Vol. 8B; Marsh, K. N., Ed.; Springer: Berlin, Germany, 1996.

(29) Suri, S. Thermodynamic properties of solutions containing an aliphatic amine. 2. Excess volumes of binary mixtures of triethylamine with 12 hydrocarbons at 313.15 K. *J. Chem. Eng. Data* **1980**, *25*, 390−393.

(30) Fermeglia, M.; Torriano, G. Density, viscosity, and refractive index for binary systems of n-C16 and four nonlinear alkanes at 298.15 K. *J. Chem. Eng. Data* **1999**, *44*, 965−969.

(31) Steiger, M.; Boissonnas, C. G.; Gernandez-Garcia, J. G. Thermodynamics of binary liquid mixtures. Volume of mixing of normal and branched alkanes. *Helv. Chim. Acta* **1972**, *55*, 1329−1333.

(32) Chi, H.; Li, G.; Guo, Y.; Fang, W. Excess molar volume along with viscosity, flash point and refractive index for binary mixtures of cis-decalin or trans-decalin with C$_9$ to C11 n-alkanes. *J. Chem. Eng. Data* **2013**, *58*, 2224−2232.

(33) Sanin, P. I.; Melenteva, N. V. The effect of hydrocarbon structure on viscosity. *Tr. Inst. Nefti Akad. Nauk SSSR* **1959**, *13*, 58−79.

(34) McAllister, R. A. The viscosity of liquid mixtures. *AIChE J.* **1960**, *6*, 427−431.

(35) Tat, M. E.; van Gerpen, J. H. Effect of temperature and pressure on the speed of sound and isentropic bulk modulus of mixtures of biodiesel and diesel fuels. *J. Am. Oil Chem. Soc.* **2003**, *80*, 1127−1130.

(36) Catoire, L.; Naudet, V. A unique equation to estimate flash points of selected pure liquids, Application to the correction of probably erroneous flash point values. *J. Phys. Chem. Ref. Data* **2004**, *33*, 1083−1111.

(37) NIST Standard Reference Database 69: *NIST Chemistry WebBook*, accessed via http://webbook.nist.gov/chemistry (accessed July 16, 2013).

(38) Majer, V., Svoboda, V. *Enthalpies of vaporization of organic compounds: A critical review and data compliation*; Backwell Scientific Publications: Oxford, 1985; p 300.