

Surrogate Mixture Model for the Thermophysical Properties of Synthetic Aviation Fuel S-8: Explicit Application of the Advanced Distillation Curve

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Fluid volatility is an important property of liquid fuels that previously has not been adequately addressed in the development of surrogate models for the thermophysical properties of these fluids. Especially important and timely is the development of surrogates for aviation fuels. In the present context, models refer to mathematical descriptions such as equations of state that provide a predictive capability. In this work, we demonstrate how the incorporation of volatility data, in the form of a distillation curve, leads to the development of improved surrogate models for aviation fuels. As an example, we present a seven-component surrogate mixture model for the thermophysical properties of a natural gas derived, synthetic aviation fuel known as S-8. We then compare the properties of the surrogate model with experimental density, sound speed, viscosity, thermal conductivity, and distillation curve data for the real fuel.

Introduction

Fuel Surrogates. The production of aviation fuel in the United States is approximately 1.65 million barrels per day (1.65×10^6 bbl/day).¹ Because of environmental concerns and issues related to energy security and fuel availability, there is a great deal of interest in alternative fuels for aviation. Synthetic fuels derived from natural gas, coal, or other hydrocarbon feedstocks are of particular interest because there is the potential of integrating them into existing aircraft with minimal modifications to the current aircraft engine designs.² One such fuel made from natural gas is known as S-8 (the “S” referring to synthetic; CAS No. 437986-20-4).³ This fluid, intended as a synthetic substitute for JP-8 (which is currently the most common military aviation fuel), is a hydrocarbon mixture rich in C7 to C18 linear and branched alkanes.⁴ It has a flash point range of between 37.8 and 51.8 °C, an autoignition temperature of 210 °C, and explosive limits in air between 0.7 and 5% (v/v). It is clear in appearance (no dye is added to current formulations).

Because this is a relatively new fuel, engine designers and manufacturers must tailor the operating parameters to suit the fluid; otherwise, the engine might require de-rating in terms of operating life. This optimization process requires a substantial input of reliable information concerning the applicability and behavior of this fuel. Important among the requirements is an understanding of the fluid thermophysical properties, because

such properties are critical for engine design and operation. Because S-8 is a complex mixture of several hundred components (summarized in Table 1),⁴ modeling its properties using a mixture model with equations for all of the constituents in the mixture is not a practical solution.

An alternative approach is to model these properties of the fuel with a surrogate mixture.

Depending upon the application for which the surrogate fuel is intended, a single pure fluid (for example, in modeling injection of jet fuel at supercritical conditions⁵) or a mixture of as many as 34 components⁶ may have to be used. Edwards and Maurice⁷ reviewed some of the surrogates available for aviation and rocket fuels; that paper provides an overview of the general requirements and expectations of fuel surrogates. Our goal in this work is to demonstrate the use of advanced distillation curve measurements to improve the volatility characteristics of a surrogate model to better represent the thermodynamic and transport properties of the actual S-8 fluid. The desire is to represent the fluid properties to within the uncertainty of the available experimental data. Moreover, we desire a surrogate mixture containing between 5 and 10 components that can be easily implemented for engineering calculations. Note that this mixture is not intended to be a surrogate for soot formation⁸ or pool fire simulations⁹ or a chemical kinetic model;^{10,11} we

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(1) Energy Information Administration (EIA), Annual Energy Review 2006, Report No. DOE/EIA-0384(2006). <http://www.eia.doe.gov/emeu/aer/txt/ptb0511.html> (accessed July 2, 2007).

(2) Daggett, D.; Hadaller, O.; Hendricks, R.; Walther, R. *Alternative Fuels and Their Potential Impact on Aviation*; NASA/TM-2006-214365; NASA: Cleveland, OH, 2006.

(3) *MSDS S-8 synthetic jet fuel, material safety data sheet*; Syntroleum Corp.: Tulsa, OK, 2005.

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

(5) Doughty, T.; Ervin, J. S.; Williams, T. F.; Bento, J. Studies of injection of jet fuel at supercritical conditions. *Ind. Eng. Chem. Res.* **2002**, *41*, 5856–5866.

(6) Dietzel, K. D.; Campbell, J. L.; Bartlett, M. G.; Witten, M. L.; Fisher, J. W. Validation of a gas chromatography/mass spectrometry method for the quantification of aerosolized Jet Propellant 8. *J. Chromatogr., A* **2005**, *1093* (1–2), 11–20.

(7) Edwards, T.; Maurice, L. Q. Surrogate mixtures to represent complex aviation and rocket fuels. *J. Propul. Power* **2001**, *17* (2), 461–466.

(8) Yan, S. H.; Jiang, Y. J.; Marsh, N. D.; Eddings, E. G.; Sarofim, A. F.; Pugmire, R. J. Study of the evolution of soot from various fuels. *Energy Fuels* **2005**, *19* (5), 1804–1811.

(9) Eddings, E. G.; Yan, S. H.; Ciro, W.; Sarofim, A. F. Formulation of a surrogate for the simulation of jet fuel pool fires. *Combust. Sci. Technol.* **2005**, *177* (4), 715–739.

Table 1. Listing of the Major Components That Were Identified in the Sample of S-8 Used for the Distillation Curve Measurements^a

name	CAS No.	area percentage
2-methylheptane	592-27-8	0.323
3-methylheptane	589-81-1	0.437
1,2,3-trimethylcyclopentane	15890-40-1	0.965
2,5-dimethylheptane	2216-30-0	1.131
4-methyloctane	2216-34-4	2.506
3-methyloctane	2216-33-3	1.323
<i>n</i> -nonane	111-84-2	1.623
3,5-dimethyloctane	15869-96-9	1.035
2,6-dimethyloctane	2051-30-1	0.756
4-ethyloctane	15869-86-0	1.032
4-methylnonane	17301-94-9	1.904
2-methylnonane	871-83-0	1.019
3-methylnonane	5911-04-6	1.385
<i>n</i> -decane	124-18-5	2.050
2,5-dimethylnonane	17302-27-1	1.175
5-ethyl-2-methyloctane	62016-18-6	1.015
5-methyldecane	13151-35-4	1.315
4-methyldecane	2847-72-5	1.134
2-methyldecane	6975-98-0	1.529
3-methyldecane	13151-34-3	1.583
<i>n</i> -undecane	1120-21-4	2.420
<i>x</i> -methylundecane	NA	1.590
3-methylundecane	1002-43-3	1.15
5-methylundecane	1632-70-8	1.696
4-methylundecane	2980-69-0	1.045
2-methylundecane	7045-71-8	1.072
2,3-dimethylundecane	17312-77-5	1.213
<i>n</i> -dodecane	112-40-3	2.595
4-methyldodecane	6117-97-1	0.929
<i>x</i> -methyldodecane	NA	0.744
2-methyldodecane	1560-97-0	1.293
<i>x</i> -methyldodecane	NA	1.281
<i>n</i> -tridecane	629-50-5	1.739
4-methyltridecane	26730-12-1	0.836
6-propyltridecane	55045-10-8	1.052
<i>x</i> -methyltridecane	NA	1.066
<i>n</i> -tetradecane	629-59-4	1.562
<i>x</i> -methyltetradecane	NA	1.198
5-methyltetradecane	25117-32-2	0.720
<i>n</i> -pentadecane	629-62-9	1.032
<i>x</i> -methyltetradecane	NA	0.727

^a Major peaks include those with a measured uncorrected area count above 1% of the total for the sample; less abundant peaks were included in this compilation to adequately cover the light and heavy ends, for modeling.

concern ourselves here only with the thermophysical properties. Following an approach presented in an earlier work¹² on the rocket propellant RP-1, we develop a surrogate model using both thermodynamic properties (density, sound speed, and boiling point) and transport properties (thermal conductivity and viscosity), but in addition, we incorporate results from recent

(10) Violi, A.; Yan, S.; Eddings, E. G.; Sarofim, F.; Granata, S.; Faravelli, T.; Ranzi, E. Experimental formulation and kinetic model for JP-8 surrogate mixtures. *Combust. Sci. Technol.* **2002**, *174* (11–2), 399–417.

(11) Ranzi, E. A Wide-Range Kinetic Modeling Study of Oxidation and Combustion of Transportation Fuels and Surrogate Mixtures. *Energy Fuels* **2006**, *20* (3), 1024–1032.

(12) Magee, J. W.; Bruno, T. J.; Friend, D. G.; Huber, M. L.; Laesecke, A.; Lemmon, E. W.; McLinden, M. O.; Perkins, R. A.; Baranski, J.; Widegren, J. A. *Thermophysical Properties Measurements and Models for Rocket Propellant RP-1: Phase I*; NIST: Boulder, CO, 2007.

(13) Bruno, T. J. Improvements in the Measurement of Distillation Curves. 1. A Composition-Explicit Approach. *Ind. Eng. Chem. Res.* **2006**, *45*, 4371–4380.

(14) Bruno, T. J. Method and apparatus for precision in-line sampling of distillate. *Sep. Sci. Technol.* **2006**, *41* (2), 309–314.

(15) Bruno, T. J.; Smith, B. L. Enthalpy of combustion of fuels as a function of distillate cut: Application of an advanced distillation curve method. *Energy Fuels* **2006**, *20* (5), 2109–2116.

advancements in the measurement of distillation curves^{4,13–18} to allow a better representation of the volatility characteristics of the fuel.

Distillation Curves. It is clearly not practical to include a rigorous description of vapor–liquid equilibria (VLE) in a surrogate mixture model without access to a huge quantity of measured VLE data (for binaries of the surrogate constituents and the overall surrogate). This goal can be approached in an approximate fashion by a measure of the overall fluid volatility, however. The distillation curve of complex multicomponent fluids has traditionally been the avenue by which complex fluid volatility has been described, usually by application of the metrology described in ASTM D-86.¹⁹ Indeed, there is invariably a section called “volatility” or “distillation” present on the specification sheets of all fuels that reports ASTM D-86 results. In this context, the distillation curve is a graphical depiction of the boiling temperature of the fluid plotted against the volume or the volume fraction. Unfortunately, the classical application of this distillation curve measurement method, while standardized, has no basis in theory and cannot be used to represent thermodynamic state points. To remedy this problem, we have developed the advanced distillation curve metrology that has been described previously.^{4,13–18} This new 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) corrosivity assessment of each distillate fraction. While all of these capabilities have been implemented on the advanced distillation curve metrology, there is no need to apply all of them in every situation. Thus, in the measurement of a low sulfur diesel fuel, for example, there would be no need to measure the corrosivity of each fraction. The apparatus for this metrology is illustrated schematically in Figure 1. Because the operation of the apparatus has been described fully elsewhere, additional operational details will not be provided here.

This approach also provides important advantages over other methods such as the simulated distillation method embodied in procedures such as ASTM D-2887. In that method, one uses the gas chromatographic behavior of a suite of compounds as a frame of comparison with a fuel. This method, while useful, is not standardized and cannot be used for equation of state development.

As pointed out in earlier work,¹³ the specific location of the thermocouple in the liquid in the boiling flask or kettle, T1 in Figure 1, allows the process to be modeled, because it represents a thermodynamic state point, and is easily reproducible and

(16) Smith, B. L.; Bruno, T. J. Advanced distillation curve measurement with a model predictive temperature controller. *Int. J. Thermophys.* **2006**, *27* (5), 1419–1434.

(17) Smith, B. L.; Bruno, T. J. Improvements in the measurement of distillation curves. 3. Application to gasoline and gasoline plus methanol mixtures. *Ind. Eng. Chem. Res.* **2007**, *46* (1), 297–309.

(18) Smith, B. L.; Bruno, T. J. Improvements in the measurement of distillation curves. 4. Application to the aviation turbine fuel Jet-A. *Ind. Eng. Chem. Res.* **2007**, *46* (1), 310–320.

(19) *Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure*; ASTM Standard D 86-04b.; American Society for Testing and Materials: West Conshohocken, PA, 2004.

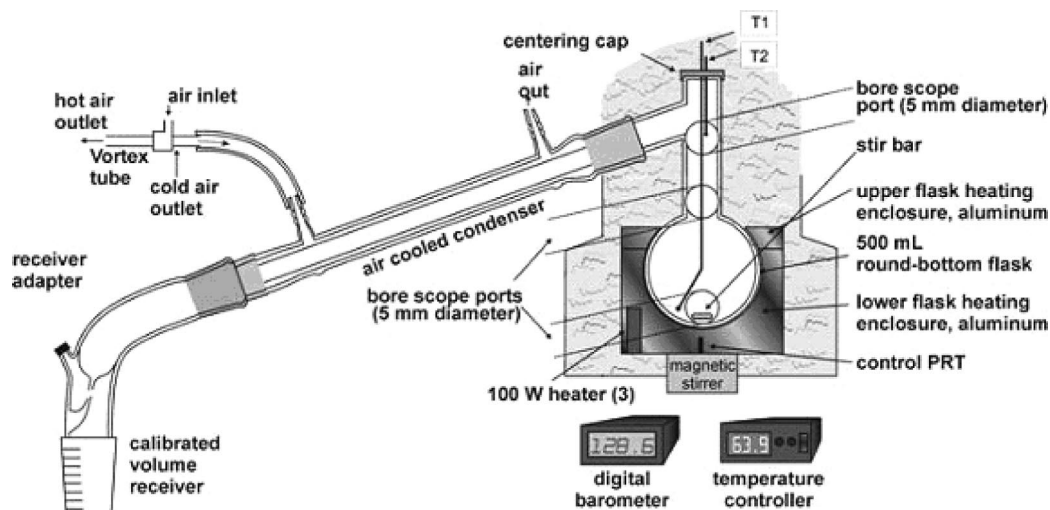


Figure 1. Schematic diagram of the overall apparatus used for the measurement of the distillation curves. Note that the bore scope observation ports are only 5 mm in diameter. The size is exaggerated on the figure to make the location clear.

preferable to the head temperature, which is very sensitive to placement in the apparatus as well as the heating rate.¹³

Theory

We can model the distillation process as a simple batch distillation,^{20,21} where the vapor leaving the boiling flask and head passes into a total condenser without reflux. The liquid in the kettle is assumed to be heated to its bubble point, and it is assumed to be in equilibrium with its vapor phase. The vapor is subsequently removed at a constant flow rate. For our theoretical description of the measurement, the vapor–liquid equilibrium for the system is represented with a mixture model^{22,23} which incorporates high accuracy Helmholtz equations of state and mixing rules with estimated interaction parameters.²⁴ These equations and mixing rules are implemented in the NIST REFPROP computer program²⁵ and will be described in more detail later in this paper.

In our approach, to model the thermophysical properties of a surrogate mixture, an equation of state and a viscosity and thermal conductivity surface for each pure fluid is required. We use mixtures of real components, similar to the method suggested by Eckert and Vanek,^{26,27} instead of pseudocompo-

nents as is common in the petroleum industry. For nonpolar hydrocarbons, simple cubic equations of state such as the Peng–Robinson²⁸ or a variant of the Statistical Associating Fluid Theory (SAFT) equation²⁹ (although the association term is unnecessary for the fluids in this work) are applicable.

In this work, we use the “short” Span–Wagner equation of state³⁰ in which the Helmholtz energy is expressed as the sum of an ideal gas term and a residual Helmholtz energy term. This energy is written as an expansion in terms of reduced density and temperature, with the critical temperature and critical density of the fluid as the primary reducing properties. This form was developed with data from several simple hydrocarbons, such as the normal alkanes methane through *n*-octane, isobutene, cyclohexane, and several other nonpolar fluids, and is expected to apply well to fluids in this study. In addition, the NIST TDE database^{31,32} can generate the coefficients automatically in a format that is easily incorporated into the REFPROP²⁵ computer program that we use for our mixture modeling, discussed in the next section. For fluids with limited data, predicted property data can be easily incorporated into the equation development. Viscosity and thermal conductivity surfaces for each of the pure constituent fluids were developed using experimental data, predictive methods, and an extended corresponding states model³³ using *n*-dodecane as the reference fluid.^{34,35} The resultant estimated uncertainty for the pure fluid models is dependent upon the experimental data used in the development of the equations; in general, the uncertainty for the liquid density

(20) Kister, H. Z. *Distillation Design*; McGraw-Hill Inc.: New York, 1992.

(21) Geankoplis, C. J. *Transport Processes and Unit Operations*, 3rd ed.; Prentice Hall: Englewood Cliffs, NJ, 1993.

(22) Kunz, O.; Klimeck, R.; Wagner, W.; Jaeschke, M. *The GERG-2004 Wide-Range Reference Equation of State for Natural Gases and Other Mixtures*; GERG Technical Monograph Fortsch.-Ber. VDI; VDI-Verlag: Dusseldorf, Germany, 2007.

(23) Lemmon, E. W.; Jacobsen, R. T. A Generalized Thermodynamic Model for the Thermodynamic Properties of Mixtures. *Int. J. Thermophys.* **1999**, *20* (3), 825–835.

(24) Lemmon, E. W.; McLinden, M. O. Method for Estimating Mixture Equation of State Parameters. *Proceedings of the Thermophysical Properties and Transfer Processes of New Refrigerants Conference*, Paderborn, Germany, 2001; International Institute of Refrigeration Commission B1: Paderborn, Germany, 2001; pp 23–30.

(25) NIST Standard Reference Database 23, *NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)*, Version 8.0; Standard Reference Data; National Institute of Standards and Technology: Gaithersburg, MD, 2007.

(26) Eckert, E.; Vanek, T. Extended utilization of the characterization of petroleum mixtures based on real components. *Chem. Pap. (Chemicke Zvesti)* **2005**, *59* (6A), 428–433.

(27) Eckert, E.; Vanek, T. New approach to the characterisation of petroleum mixtures used in the modelling of separation processes. *Comput. Chem. Eng.* **2005**, *30* (2), 343–356.

(28) Peng, D.; Robinson, D. B. New 2-Constant Equation of State. *Ind. Eng. Chem. Fundam.* **1976**, *15* (1), 59–64.

(29) Gross, J.; Sadowski, G. Perturbed-chain SAFT: An equation of state based on a perturbation theory for chain molecules. *Ind. Eng. Chem. Res.* **2001**, *40* (4), 1244–1260.

(30) Span, R.; Wagner, W. Equations of state for technical applications. I. Simultaneously optimized functional forms for nonpolar and polar fluids. *Int. J. Thermophys.* **2003**, *24* (1), 1–39.

(31) NIST Standard Reference Database 103, *NIST ThermoData Engine*, Version 2.0; Standard Reference Data; National Institute of Standards and Technology: Gaithersburg, MD, 2006.

(32) Muzny, C. D.; Lemmon, E. W.; Chirico, R. D.; Diky, V.; Dong, Q.; Frenkel, M. Dynamic equation of state evaluation with ThermoData Engine. *Abstr. Pap. Am. Chem. Soc.* **2005**, *230*, U1008–U1008.

(33) Huber, M. L.; Laesecke, A.; Perkins, R. A. Model for the Viscosity and Thermal Conductivity of Refrigerants, Including a New Correlation for the Viscosity of R134a. *Ind. Eng. Chem. Res.* **2003**, *42*, 3163–3178.

(34) Lemmon, E. W.; Huber, M. L. Thermodynamic properties of *n*-dodecane. *Energy Fuels* **2004**, *18* (4), 960–967.

(35) Huber, M. L.; Laesecke, A.; Perkins, R. Transport properties of *n*-dodecane. *Energy Fuels* **2004**, *18* (4), 968–975.

for typical fuel constituent fluids is on the order of 3%, for the vapor pressures from 1 to 5%, and for the viscosity and thermal conductivity approximately 5–10%.

For calculations of the thermodynamic properties of mixtures, we use a mixture model explicit in the Helmholtz energy that can utilize any equation of state, provided that it can be expressed in terms of the Helmholtz energy.³⁶ This form of the model has been used successfully for refrigerant mixtures³⁶ and for natural gas mixtures.²² The basic idea is to represent the molar Helmholtz energy, a , of a mixture as a sum of an ideal solution contribution a^{idsol} and an excess contribution a^{excess} according to the following:

$$a = a^{\text{idsol}} + a^{\text{excess}} \quad (1)$$

$$a^{\text{idsol}} = \sum_{j=1}^m x_j [a_i^0(\rho, T) + a_i^r(\delta, \tau) + RT \ln x_j] \quad (2)$$

$$a^{\text{excess}} = RT \sum_{i=1}^{m-1} \sum_{j=i+1}^m x_i x_j F_{ij} \sum_k N_k \delta^{d_k} \tau^{l_k} \exp(-\delta^{l_k}) \quad (3)$$

where ρ and T are the mixture molar density and temperature, δ and τ are the reduced mixture density and temperature, m is the number of components, a_i^0 is the ideal gas Helmholtz energy of component i , a_i^r is the residual (or real fluid) Helmholtz energy of component i , the x_i are the mole fractions of the constituents of the mixture, d_k , t_k , l_k , and N_k are coefficients found from fitting experimental data, and F_{ij} is an interaction parameter. Mixing rules are used to determine the reducing parameters ρ_{red} and T_{red} for the mixture that are defined as

$$\delta = \rho / \rho_{\text{red}} \quad (4)$$

$$\tau = T_{\text{red}} / T \quad (5)$$

$$\rho_{\text{red}} = \left[\sum_{i=1}^m \frac{x_i}{\rho_{c_i}} + \sum_{i=1}^{m-1} \sum_{j=i+1}^m x_i x_j \xi_{ij} \right]^{-1} \quad (6)$$

$$T_{\text{red}} = \sum_{i=1}^m x_i T_{c_i} + \sum_{i=1}^{m-1} \sum_{j=i+1}^m x_i x_j \zeta_{ij} \quad (7)$$

where ξ_{ij} and ζ_{ij} are the binary interaction parameters that define the shapes of the reducing temperature and density curves.

The model has a total of three binary interaction parameters, ξ_{ij} , ζ_{ij} , and F_{ij} , that can be determined by fitting experimental data when available. Because the constituent fluids in this work are chemically similar, we set the excess contribution to zero (i.e., $F_{ij} = 0$) and the ξ_{ij} interaction parameter to zero, resulting in a simpler model with only one binary interaction parameter, ζ_{ij} . Previous studies on refrigerant mixtures have shown that ζ_{ij} is the most important binary parameter. This parameter can be found by fitting binary mixture data, or when data are unavailable, as is the case in this work, the following predictive scheme is used²⁴

$$\zeta_{ij} = \frac{T_{c_2}}{T_{c_1}} (40.4 - 25.03 \times 2^s) \quad (8)$$

$$s = \left(\frac{T_{c_1} P_{c_2} \omega_2}{T_{c_2} P_{c_1} \omega_1} \right) \quad (9)$$

where the fluid with the smaller dipole moment is designated as fluid “1”, and ω is the acentric factor. This scheme was

(36) Lemmon, E. W.; Jacobsen, R. T. Equations of State for Mixtures of R-32, R-125, R-134a, R-143a, and R-152a. *J. Phys. Chem. Ref. Data* **2004**, *33* (2), 593–620.

developed with a database of mixture data primarily for refrigerant mixtures and resulted in average absolute deviations (AADs) of 4.5% in bubble point pressure and 1.7% in density; we anticipate similar results for the fluid mixtures in this study.

The model for calculating the transport properties of a mixture is an extended corresponding states method.^{33,37–41} The basic procedure is based upon the earlier work of Ely and Hanley.^{42,43} In this approach, the viscosity or thermal conductivity of a mixture is calculated in a two-step procedure. First, mixing and combining rules are used to represent the mixture in terms of a hypothetical pure fluid, and then, the properties of the hypothetical pure fluid are determined by mapping onto a reference fluid through the use of “shape factors”; details are given elsewhere.^{33,37–41} For both refrigerant mixtures and mixtures of natural gas components the viscosity and thermal conductivity are typically represented to within 5–10%,³⁷ and we expect similar results with the fluid mixtures in this work.

The two models discussed briefly above, the Helmholtz energy mixing model for thermodynamic properties and the extended corresponding states model for viscosity and thermal conductivity, are implemented in the REFPROP computer program.²⁵ This program contains highly accurate equations of state for pure fluids, including some that have been adopted as international standards.^{44–46} Moreover, REFPROP has been adopted as a de facto standard in the refrigeration industry. The most recent version contains a model under consideration as an international standard for the calculation of the thermodynamic properties of natural gas mixtures²² incorporating a form of the Helmholtz energy mixing model described above. In this work, we added the ability to compute the thermodynamic and transport properties of the candidate fluids listed in Table 2 to the REFPROP program and use it in all calculations because it already contains all the algorithms necessary to compute phase equilibrium (bubble points) and thermophysical properties.

Experimental Section

To initiate the development of the procedure to incorporate the distillation curve into the surrogate model development, we

(37) Chichester, J.; Huber, M. L. *Extended Corresponding States Model for Viscosity and Thermal Conductivity of Pure Fluids and Their Mixtures as Implemented in REFPROP*, Version 8; NIST IR 6650; National Institute of Standards and Technology: Boulder, CO, in preparation.

(38) McLinden, M. O.; Klein, S. A.; Perkins, R. A. An Extended Corresponding States Model for the Thermal Conductivity of Pure Refrigerants and Refrigerant Mixtures. *Int. J. Refrig.* **2000**, *23* (1), 43–63.

(39) Klein, S. A.; McLinden, M. O.; Laesecke, A. An Improved Extended Corresponding States Method for Estimation of Viscosity of Pure Refrigerants and Mixtures. *Int. J. Refrig.* **1997**, *20* (3), 208–217.

(40) Huber, M. L.; Ely, J. F. Prediction of the Viscosity of Refrigerants and Refrigerant Mixtures. *Fluid Phase Equilib.* **1992**, *80*, 239–248.

(41) Huber, M. L.; Ely, J. F. Prediction of the Thermal Conductivity of Refrigerants and Refrigerant Mixtures. *Fluid Phase Equilib.* **1992**, *80*, 249–261.

(42) Ely, J. F.; Hanley, H. J. M. Prediction of transport properties. 1. Viscosity of fluids and mixtures. *Ind. Eng. Chem. Fundam.* **1981**, *20* (4), 323–332.

(43) Ely, J. F.; Hanley, H. J. M. Prediction of transport properties. 2. Thermal conductivity of pure fluids and mixtures. *Ind. Eng. Chem. Fundam.* **1983**, *22* (1), 90–97.

(44) Wagner, W.; Pruss, A. The IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. *J. Phys. Chem. Ref. Data* **2002**, *31* (2), 387–535.

(45) Tillner-Roth, R.; Baehr, H. D. An International Standard Formulation for the Thermodynamic Properties of 1,1,1,2-Tetrafluoroethane (HFC-134a) for Temperatures from 170 to 455 K and Pressures up to 70 MPa. *J. Phys. Chem. Ref. Data* **1994**, *23* (5), 657–730.

(46) Tillner-Roth, R.; Yokozeki, A. An International Standard Equation of State for Difluoromethane (R-32) for Temperatures from the Triple Point at 136.34 to 435 K and Pressures up to 70 MPa. *J. Phys. Chem. Ref. Data* **1997**, *26* (6), 1273–1328.

Table 2. List of Potential Fluids for Inclusion in the Surrogate Mixture

fluid name	number of carbons	boiling point (K) at pressure 83 kPa
3-methylheptane	8	385
<i>n</i> -octane	8	391
2,5-dimethylheptane	9	401
<i>n</i> -nonane	9	416
4-methylnonane	10	431
2,6-dimethyloctane	10	426
<i>n</i> -decane	10	440
3-methyldecane	11	455
2,5-dimethylnonane	11	442
<i>n</i> -undecane	11	461
5-methylundecane	12	460
<i>n</i> -dodecane	12	481
2-methyldodecane	13	474
2,3-dimethylundecane	13	470
<i>n</i> -tridecane	13	500
3-methyltridecane	14	518
<i>n</i> -tetradecane	14	518
<i>n</i> -pentadecane	15	534
<i>n</i> -hexadecane	16	551

performed distillation curve measurements on two binary mixtures of *n*-decane and *n*-tetradecane (75/25 and 50/50 mol/mol %) in addition to the actual S-8 aviation fuel. The measurements were performed according to the procedure described earlier (using the apparatus shown in Figure 1), with one modification to the procedure. In addition to the usual temperature and volume channels, we also measured a time channel. Thus, starting at the vapor rising temperature¹³ (shown to be the initial boiling temperature of the mixture and recorded as time = 0), the time was recorded in addition to the temperature and volume. This allowed us to explicitly measure a rate of mass transfer through the distillation head along with the traditional distillation curve.

The *n*-decane and *n*-tetradecane used in this work were reagent grade fluids with stated purities of 99+%. The purities of these fluids were verified by an analysis using gas chromatography (GC, 30 m capillary column of 5% phenyl dimethyl polysiloxane having a thickness of 1 μ m, temperature program from 90 to 275 °C, 9 °C/min) using flame ionization detection and mass spectrometric detection.^{47,48} The synthetic aviation fuel S-8 was obtained from the United States Air Force, Air Force Research Laboratory, Propulsion Directorate, and was used without treatment or purification. Care was taken to minimize the exposure of the fluid to the atmosphere to minimize oxidation, evaporation of the more volatile components, and the uptake of moisture. A detailed chemical analysis was done to characterize this fluid.⁴ In addition, a total sulfur analysis was done on the S-8 with a gas chromatograph that was equipped with a sulfur chemiluminescence detector (SCD). Moreover, a copper strip corrosion test (CSCT) was performed. The results of the SCD and CSCT indicated that the sample was very low in sulfur. The results from the GC-SCD measurements showed that the sulfur peaks were nearly at the detection limit of the instrument/method, at 100 ppb (0.000 01 mol/mol %). Exposed copper strips recovered from the CSCT were indistinguishable from pristine strips.

Each distillation curve was measured starting with 200 mL of fluid. The uncertainties in temperature, volume, and atmospheric pressure are discussed elsewhere.^{13,14,17,18} In all of our previous presentations of distillation curve measurements, we have corrected the temperatures to standard atmospheric pressure with the modified Sidney–Young equation,¹³ although the actual experimental pressures are always provided. The reason for this is that the user community universally applies and interprets distillation curves that

have been corrected to standard atmospheric pressure. In this paper, and in surrogate model development in general, we do not apply the Sidney–Young equation; rather, we directly use the measured experimental temperatures (corrected for calibration) and the experimental pressure, along with their respective uncertainties.

Results and Discussion

We developed and tested the procedure to incorporate the distillation curve into the mixture model development process on a binary mixture of known composition, a mixture of 75/25 mol % *n*-decane and *n*-tetradecane. This mixture was selected for its simplicity and availability of thermophysical property data and because it was studied thoroughly in previous work.¹³ The resulting calculated and observed distillation curves (expressed as kettle temperature vs volume fraction collected in the receiver) are shown in Figure 2a.

We used a simple procedure to model the distillation curve. The process begins by assuming that the distillation flask contains 200 mL of liquid of a known composition and pressure and the receiver is completely empty. The pressure is assumed constant, and a bubble-point calculation is made to determine the bubble-point temperature and the compositions of the resulting equilibrium vapor phase. The entire distillation procedure for a volume of 200 mL is divided into a fixed number of volume increments, with a constant volume of fluid removed from the still at each volume step. The size of the volume step is selected to be small enough that the results are not dependent upon the step size but large enough to prevent a burdensome computation time. The vapor is then removed from the system and transferred to the receiver, where its liquid density and volume are calculated. This requires another bubble-point calculation to determine the density (and volume) of the liquid phase that results when the vapor is condensed at the known pressure. A new liquid feed in the still is then computed, and the process is repeated until a negligible volume of the liquid remains in the still. Alternatively, one could think of this as a process that is divided into a fixed number of time increments, under constant flow conditions, again resulting in a fixed volume removed at each time step. However, time does not explicitly appear in this very idealized procedure because we assume that the vapor and liquid are always intimately in contact, there are no flow, mass, or heat transfer effects, and equilibrium is instantaneously attained after an increment of fluid is instantaneously removed from the system.

The bubble-point calculation can be made with any equation-of-state model; we used the Helmholtz energy calculation described in the Theory section. Figure 2a shows that although the shapes of the two curves agree, there is a horizontal offset on the volume fraction axis. The offset is expected and corresponds to the transit delay in the experimental apparatus as a result of the time it takes for a volume element of fluid that is vaporized at the surface of the fluid in the kettle (where the temperature is measured) to arrive in the collecting vessel after traveling through the condenser and receiver adapter. We can shift the calculated distillation curve by a constant volume fraction, specific to the experimental apparatus, consistent with the mass flow rate through the apparatus. In particular, the feature of the apparatus that controls the shift is the length of the condenser and receiver adapter sections. This offset in time can be used to compute the delay in future experiments on the same apparatus (i.e., with the same condenser and receiver adapter), provided that the flow rate is maintained at a constant (although not necessarily the same) value. Clearly, if any changes are made in the apparatus that may affect the transit

(47) Bruno, T. J.; Svoronos, P. D. N. *CRC Handbook of Basic Tables for Chemical Analysis*, 2nd ed.; Taylor and Francis CRC Press: Boca Raton, FL, 2004.

(48) Bruno, T. J.; Svoronos, P. D. N. *CRC Handbook of Fundamental Spectroscopic Correlation Charts*; Taylor and Francis CRC Press: Boca Raton, FL, 2005.

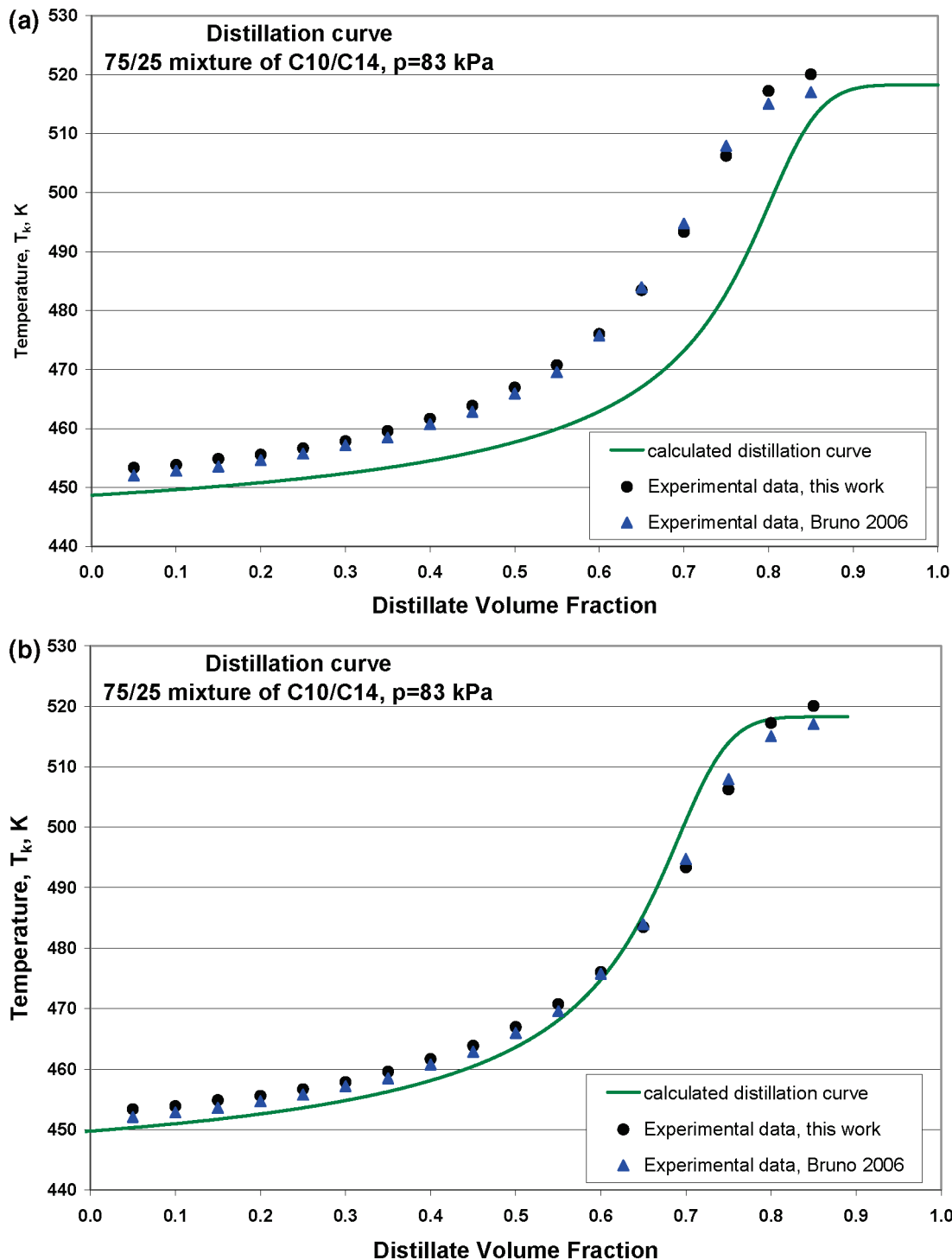


Figure 2. (a) Experimental and calculated distillation curves for a 75/25 mol fraction mixture of *n*-decane/*n*-tetradecane at 83 kPa. The offset is caused by the transit through the apparatus, as discussed in the text. (b) Experimental and calculated distillation curves for a 75/25 mol fraction mixture of *n*-decane/*n*-tetradecane at 83 kPa, adjusted for the transit volume shift. A detailed discussion of the uncertainty in these data is provided in ref 13.

period (such as changing the length of the condenser of the receiver adapter), the transit offset would have to be remeasured.

As was stated previously, the earliest measurement on the developmental apparatus¹³ was made with manual control of the flow rate and did not contain flow rate information. A later improvement in the apparatus, the introduction of the model predictive controller,¹⁶ permitted a better control of the flow rate. The experimental results performed with this controller are presented in Table 3. Figure 2b displays the calculated results adjusted with the volume shift. The volume shift was found by adjusting the value of the shift until agreement between the

calculated and the observed distillation curves was achieved. The calculated results capture much of the experimental behavior but do not agree with the experimental data exactly. The model assumes that there is no reflux and that the flow rate is constant. We also consider only the vapor–liquid equilibrium at the surface and neglect any transport effects. Deviations from these simplifying assumptions will introduce discrepancies between the experimental and the calculated results.

To provide additional verification of the calculation procedure, we repeated the previous measurements¹³ on a 50/50 mixture at an atmospheric pressure of 83.2 kPa and, in addition, made

Table 3. Distillation Curve for a 75/25 Mole Fraction Mixture of *n*-Decane and *n*-Tetradecane at a Constant Atmospheric Pressure of 83.35 kPa^a

time (min)	volume fraction	kettle temperature, T_k (K)
2.0	0.05	453.4
3.2	0.10	453.9
4.3	0.15	454.9
5.4	0.20	455.6
6.6	0.25	456.7
7.8	0.30	457.9
9.0	0.35	459.6
10.1	0.40	461.7
11.2	0.45	463.9
12.5	0.50	467.0
13.8	0.55	470.8
15.3	0.60	476.1
17.0	0.65	483.5
19.0	0.70	493.4
21.9	0.75	506.3
25.4	0.80	517.3
27.4	0.85	520.1
28.7	0.90	520.6
30.2	0.95	520.9

^a A detailed discussion of the uncertainty in these data is provided in ref 13.

Table 4. Distillation Curve for a 50/50 Mole Fraction Mixture of *n*-Decane and *n*-Tetradecane at a Constant Atmospheric Pressure of 83.2 kPa^a

time (min)	volume fraction	kettle temperature, T_k (K)
0.75	0.025	462.45
4.25	0.05	465.95
7.47	0.10	468.15
11.00	0.15	470.85
14.92	0.20	473.85
19.42	0.25	477.45
24.78	0.30	481.45
31.07	0.35	486.95
38.10	0.40	494.35
46.72	0.45	503.15
54.87	0.50	509.85
60.00	0.55	513.85
63.45	0.60	515.95
65.85	0.65	517.15
67.85	0.70	517.65
69.62	0.75	517.75
71.18	0.80	517.55
72.72	0.85	517.55
74.30	0.90	518.45
75.80	0.95	523.65

^a A detailed discussion of the uncertainty in these data is provided in ref 13.

distillation measurements on a 50/50 mol fraction mixture of *n*-decane/*n*-tetradecane at an atmospheric pressure of 70.05 kPa (the latter measurement was made at 3110 m above sea level). The results for these runs are presented in Tables 4 and 5, and the results are shown graphically in Figures 3 and 4. We selected a volume shift that gave the best agreement with the experimental curves; for the three cases in Figures 2–4, we found volume shifts of 0.10, 0.13, and 0.12 volume fraction, respectively. While there is some degree of random uncertainty involved with the determination of the shift for the instrument, the shift was relatively consistent between the three runs. We chose an average value of 0.12 to represent the constant for the apparatus which is necessary for modeling the surrogate mixture. As one form of checking the procedure, we calculated the composition of the mixture used in Figure 2b by minimizing the deviations between the predicted distillation curve obtained with a volume shift of 0.12 and the experimental curve. We calculated a decane mole fraction of 0.76; the experimental value is 0.75.

Table 5. Distillation Curve for a 50/50 Mole Fraction Mixture of *n*-Decane and *n*-Tetradecane at a Constant Atmospheric Pressure of 70.06 kPa^a

time (min)	volume fraction	kettle temperature, T_k (K)
0.00	0.025	459.35
1.77	0.05	461.15
3.15	0.10	462.95
4.73	0.15	465.45
6.38	0.20	468.05
8.10	0.25	471.15
10.23	0.30	474.95
12.50	0.35	479.15
15.25	0.40	484.25
18.68	0.45	490.75
22.02	0.50	497.25
25.12	0.55	502.95
27.70	0.60	507.15
29.83	0.65	509.75
31.50	0.70	511.05
33.05	0.75	512.15
34.12	0.80	512.35
35.13	0.85	512.35
36.07	0.90	512.25
36.95	0.95	511.75

^a A detailed discussion of the uncertainty in these data is provided in ref 13.

Finally, we measured the distillation curve of a sample of S-8 under constant volume flow conditions; these results are presented in Table 6. A distillation curve for this sample was obtained in an earlier work,⁴ and the present curve is in good agreement with the earlier work that was obtained without the model predictive controller.¹⁶

Development of the Surrogate Mixture Model for S-8. The procedure for developing a surrogate mixture for S-8 can be summarized as follows. First, a chemical analysis is performed to identify the chemical composition of the fuel sample. From this analysis, a list of representative fluids is constructed, including fluids representative of the various chemical families (branched or straight-chain alkanes, alkenes, aromatics, naphthenes, etc.) and the number of carbons of the fluids found in the sample. For each of these possible pure fluid constituents, an equation of state, viscosity, and a thermal conductivity surface are needed. If this information is not available in the literature, it must be developed from available experimental data or predictive methods. To represent the properties of a mixture, mixture models are used that incorporate the pure fluid equations for both thermodynamic and transport properties. The fluids in the surrogate mixture and their compositions are found by a multiproperty regression to determine the composition that minimizes the difference between predicted and experimental thermophysical property data for the S-8 fuel sample. The process incorporates data for density, sound speed, viscosity, thermal conductivity, and volatility (i.e., the distillation curve). The resultant surrogate mixture composition can be used to model the thermophysical properties of the S-8 fuel.

Analysis of the mixture with a gas chromatographic–mass spectrometric method revealed S-8 to be a mixture of linear and branched alkanes of 7–18 carbons, with approximately 320 peaks easily distinguishable from the noise and 25 identifiable components at a 1% area level.⁴ For each monobranched alkane identified in the chemical analysis,⁴ a representative species was selected as a candidate constituent fluid for the surrogate. In other words, for our purposes all *x*-methyldecane are represented as a single methyldecane, and similarly we used a particular *x,y*-dimethyl alkane to represent the dimethyl family. A major factor governing the specific choice of compound to represent a moiety was the availability of property data: priority

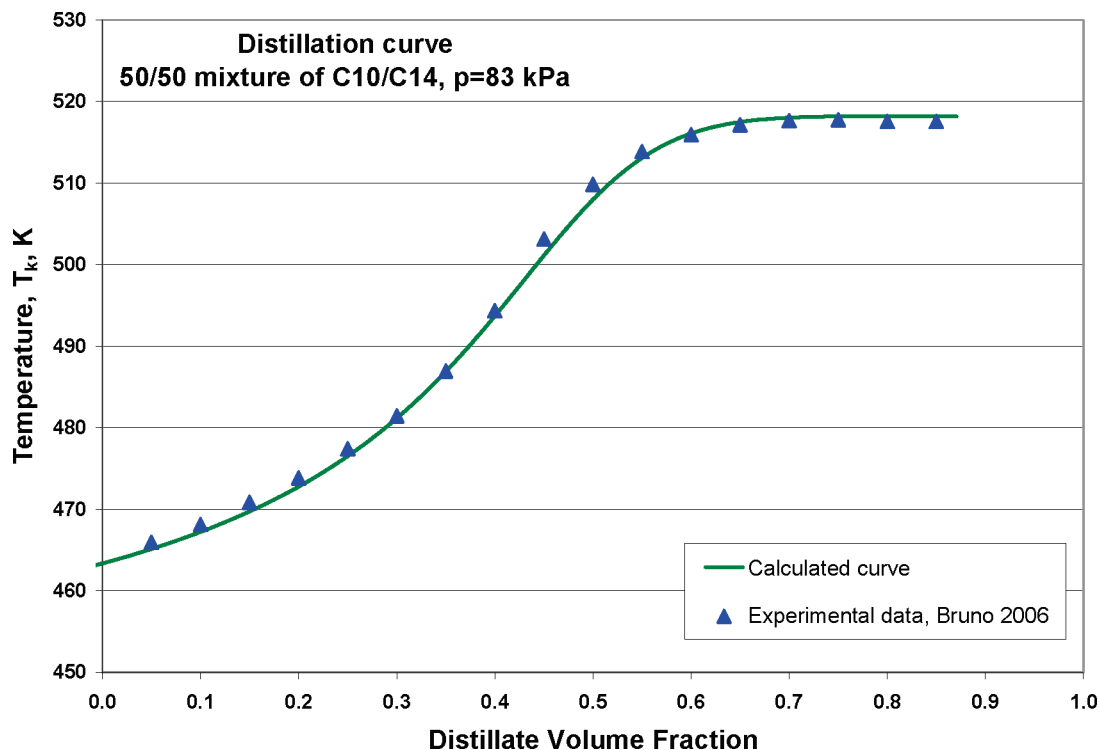


Figure 3. Experimental and calculated distillation curves for a 50/50 mol fraction mixture of *n*-decane/*n*-tetradecane at 83 kPa, adjusted for the transit volume shift. A detailed discussion of the uncertainty in these data is provided in ref 13.

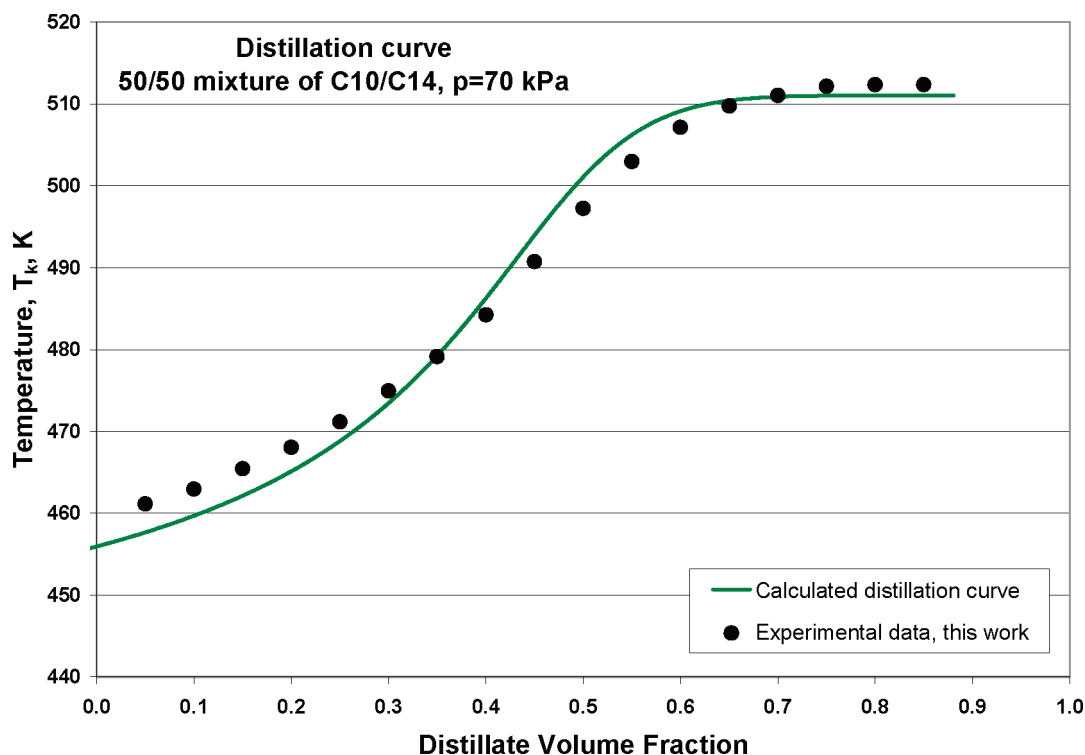


Figure 4. Experimental and calculated distillation curves for a 50/50 mol fraction mixture of *n*-decane/*n*-tetradecane at 70 kPa, adjusted for transit volume shift. A detailed discussion of the uncertainty in these data is provided in ref 13.

was given to compounds for which the most abundant and reliable experimental measurements were available. Following this procedure, for each possible constituent fluid we searched the open literature as well as databases such as NIST TDE,³¹ DIPPR,⁴⁹ and Landolt–Bornstein⁵⁰ for experimental physical

property data. For some of the branched alkanes, the data are limited and were supplemented with predicted values generated by either the DIPPR database⁴⁹ or the TDE³¹ database. Table 2 presents the list of possible constituent fluids for the S-8

(49) Rowley, J. R.; Wilding, W. V.; Oscarson, J. L.; Rowley, R. L. *DIADDEM, DIPPR Information and Data Evaluation Manager*, Version 2.0; Brigham Young University: Provo, UT, 2002.

(50) Wohlfarth, C.; Wohlfarth, B. Viscosity of Pure Organic Liquids and Binary Liquid Mixtures. *Landolt-Börnstein-Numerical Data and Function Relationships in Science and Technology, IV/18*; Springer-Verlag: Berlin, 2001; Vol. subvolume B. Pure Organic Liquids.

Table 6. Distillation Curve for S-8 at a Constant Atmospheric Pressure of 82.87 kPa^a

time (min)	volume fraction	kettle temperature, T_k (K)
1.98	0.05	453.05
3.12	0.10	455.45
4.42	0.15	458.25
5.50	0.20	461.05
6.62	0.25	463.95
7.88	0.30	466.95
9.07	0.35	470.45
10.35	0.40	473.95
10.82	0.45	477.95
13.23	0.50	481.75
14.63	0.55	486.05
16.20	0.60	491.05
17.68	0.65	495.85
19.38	0.70	501.35
20.82	0.75	506.15
22.38	0.80	511.95
24.48	0.85	519.35
27.22	0.90	528.65
32.08	0.95	541.65

^a A detailed discussion of the uncertainty in these data is provided in ref 13.

Table 7. Composition of Surrogate Mixture

fluid	mole fraction
<i>n</i> -nonane	0.03
2,6-dimethyloctane	0.28
3-methyldecane	0.34
<i>n</i> -tridecane	0.13
<i>n</i> -tetradecane	0.20
<i>n</i> -pentadecane	0.015
<i>n</i> -hexadecane	0.005

surrogate and their boiling points at an atmospheric pressure of 83 kPa (the typical local pressure).

The final step in the procedure for development of a surrogate model is to perform a multiproperty regression to determine the compositions of the surrogate fluid mixture for S-8 that minimize the deviations between the predicted property values and the experimental data. The objective function was the sum of the squared percentage differences between the experimental data⁵¹ and the predicted value for multiple properties (experimental densities, sound speeds, thermal conductivities, viscosi-

ties, and the distillation curve). The procedure is not limited to the types of data used here. Any kind of available experimental data that can be modeled, including properties such as heat capacity and surface tension that were not available for this study, can be used. Each type of property data was assigned a weight, and the weights were adjusted until the deviations for the distillation curve were less than 1%, a level we consider acceptable for design and optimization of aviation fuel applications. Other weights can be selected as well, depending on the intended goal; for example, if accurate density is the goal, one could increase the weight on density and relax the weight on the distillation curve. In addition, although not done here, one could include constraints, such as the H/C ratio. To obtain an initial guess for the slate of components, we examined the experimental distillation curve and the boiling points in Table 2 and selected fluids with boiling points to cover the range observed experimentally. The initial mixtures had as many as 10 components, but it became clear that a smaller number of components could adequately represent the properties (the regression resulted in very small mole fractions of some components). The number of constituent fluids was selected to be the minimum possible for the representation of the shape of the distillation curve.

The final surrogate composition, containing seven components, is given in Table 7. The computed distillation curve (adjusted with a volume shift of 0.12) and the experimental data are shown in Figure 5. The difference between the calculated and the experimental distillation temperatures is always within 1%; the largest deviation was 3 K at the very highest temperature, 519.35 K. The lightest (*n*-nonane) and the heaviest fluids (*n*-hexadecane) are present only in small amounts and determine the initial boiling behavior and the tail of the distillation curve. Good agreement was found between the initial boiling point observed experimentally, 449.6 K, and the calculated initial boiling point (at 82.87 kPa) of 449.42 K. The overall shape of the distillation curve is primarily due to only four major components: 2,6-dimethyloctane, 3-methyldecane, *n*-tridecane, and *n*-tetradecane. If one is interested only in reproducing the distillation curve, then it is not necessary to use the branched alkanes 2,6-dimethyloctane and 3-methyldecane; one could substitute *n*-decane and *n*-undecane and obtain excellent results.

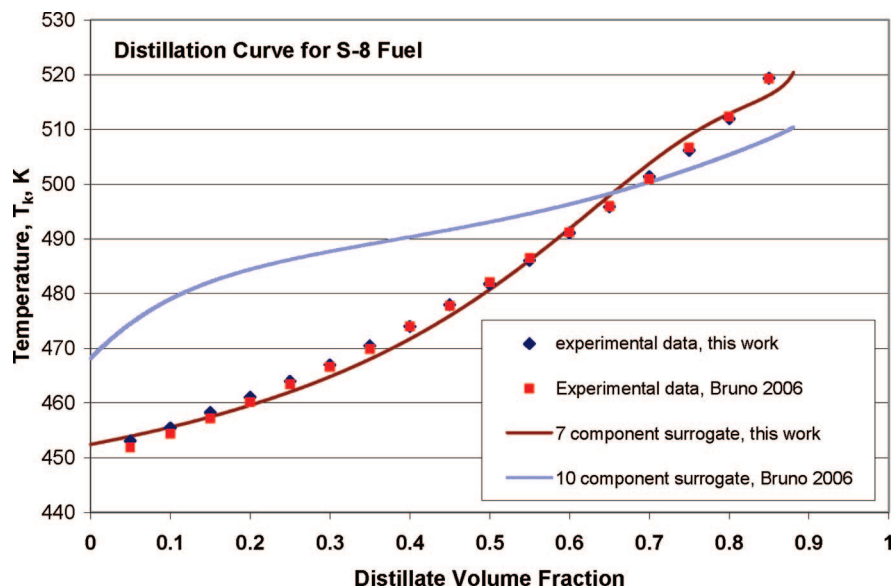


Figure 5. Experimental and calculated distillation curves for S-8 at 83 kPa, adjusted for volume shift. The curve calculated for the 10-component surrogate did not use the distillation curve of S-8 in its formulation; the curve calculated for the 7-component surrogate used the distillation curve. A detailed discussion of the uncertainty in these data is provided in ref 4.

However, this will impact the representation of some of the other properties. For example, Watanabe⁵³ studied the thermal conductivity of a series of branched alkanes and demonstrated that the thermal conductivity of the branched isomers is lower than that of the linear alkane of the same molecular weight. If the surrogate does not include branched alkanes, although the distillation curve may be represented very well, the predicted thermal conductivities will be too high.

In addition to the distillation curve, the surrogate mixture also represents the other property data very well. For 222 density data points covering the temperature range 233–470 K at pressures to 30 MPa, the AAD is 1.5%; it is 1.7% for the sound speed (35 points) at atmospheric pressure and temperatures from 278 to 343 K. The thermal conductivity (935 points) from 300 to 500 K at pressures to 70 MPa has an AAD of 1.7%, and the viscosity at atmospheric pressure (62 points) at temperatures from 233 to 373 K has an AAD of 3.5%. These values exceed the uncertainty^{51,52} of the experimental measurements for S-8 but are within the uncertainty level of the individual pure fluid correlations that are components of the mixture model. There is a lot of flexibility in the choice of the surrogate composition, depending on the properties that are given the most weight in the fitting procedure. In this work, we emphasized the reproduction of the distillation curve. Any property that can be modeled can be used in the regression and weighted accordingly to obtain a desired tolerance, resulting in many possible surrogate mixtures tailored to fit a user's requirements.

Graphical comparisons of predicted properties from the surrogate model and experimental data⁵¹ are shown in Figure 6a–d. Some of these curves appear to show systematic deviations. One possible explanation is due to inadequacies in the representation of the constituent pure fluids, especially 2,6-dimethyloctane and 3-methyldecane. The data situation for these two fluids is poor; in fact, there were no experimental data for the transport properties for these two fluids, and predictive methods were used to represent viscosity and thermal conductivity. It is quite possible that our estimates for these fluids are systematically in error. Another point is that one can achieve a better representation of the experimental data simply by adding another component to the mixture because this is equivalent to adding an additional fitting parameter. We selected seven components as an acceptable number that provided a balance between mixture complexity, computation time, and acceptable deviations from experimental data.

The surrogate has an overall average molar mass of 164.79, a hydrogen to carbon ratio (H/C) of 2.17, and an approximate chemical formula of $C_{11.6}H_{25.2}$. The overall average composition is 38% (mol/mol) straight chain alkanes and 62% branched alkanes. As mentioned previously, the sample did not contain appreciable alkenes, monocyclic paraffins, bicyclic paraffins, or aromatics; the surrogate also does not contain these classes of fluids. This mixture is a surrogate; it is not the actual mixture composition, but rather a mixture that approximates the thermophysical property behavior of the S-8 sample that was investigated.

To demonstrate the importance of including information from the distillation curve into the analysis for determining the

(51) Bruno, T. J. *The Properties of S-8*; MIPR F4FBEY6237G001, final report to sponsor WPAFB; National Institute of Standards and Technology: Boulder, CO, 2006.

(52) Bruno, T. J.; Huber, M. L.; Laesecke, A.; Lemmon, E. W.; Ott, L. S.; Outcalt, S.; Perkins, R.; Seelig, H.-D.; Smith, B. L. *The Properties of S-8*; NISTIR 6648; National Institute of Standards and Technology: Boulder, CO; in preparation.

(53) Watanabe, H. Thermal Conductivity and Thermal Diffusivity of Sixteen Isomers of Alkanes: C_nH_{2n+2} ($n=6$ to 8). *J. Chem. Eng. Data* **2003**, *48*, 124–136.

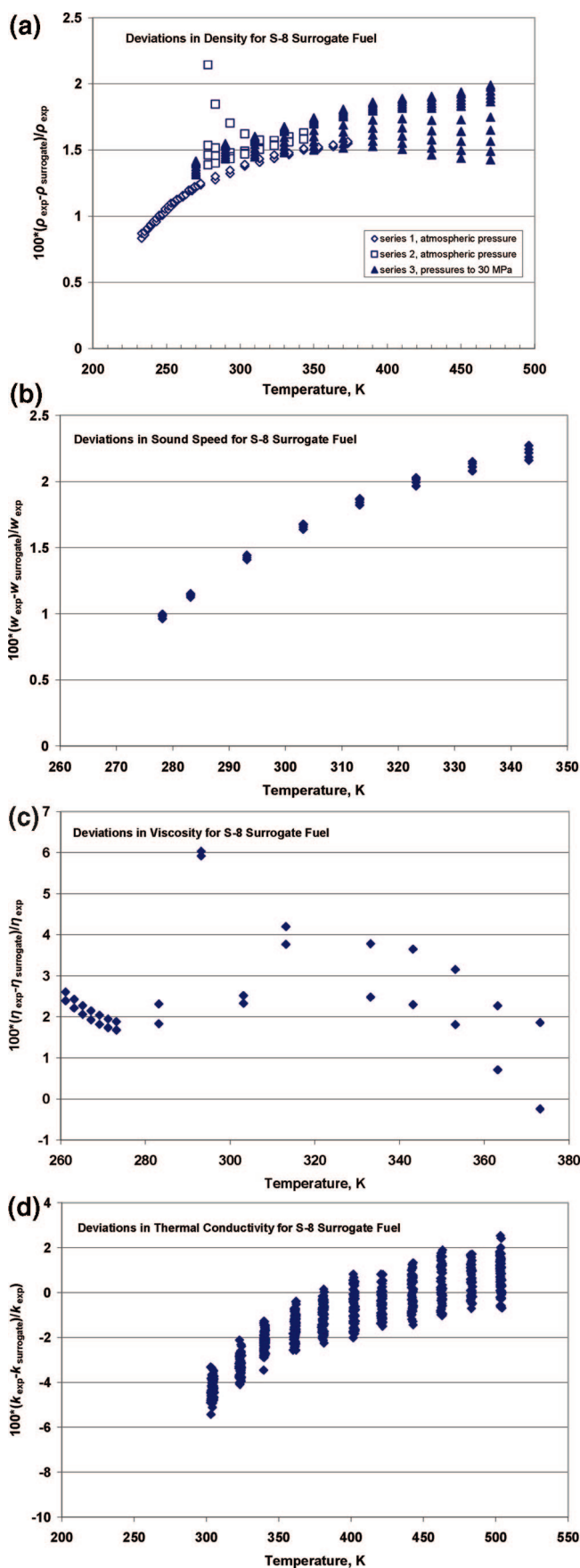


Figure 6. (a) Deviations of experimental^{51,52} and calculated surrogate density for S-8. (b) Deviations of experimental^{51,52} and calculated surrogate sound speed for S-8. (c) Deviations of experimental^{51,52} and calculated surrogate viscosity for S-8. (d) Deviations of experimental^{51,52} and calculated surrogate thermal conductivity for S-8.

composition of the surrogate, Figure 5 also shows an earlier preliminary surrogate mixture⁵¹ developed for S-8 that has 10 components but which did not take into account the distillation curve in the determination of the surrogate composition. The surrogate was determined with only density, sound speed, viscosity, and thermal conductivity data, and emphasis was placed on obtaining agreement with PVT (density) data. The shape of the earlier calculated distillation curve of the surrogate is clearly very different from the experimental curve. The difference lies not only in the temperature values (with the model predicting a much less volatile mixture than the actual fluid) but also in the slope. The experimental curve is convex while the curve predicted without the distillation curve data is concave. From this one sees that, to properly represent the volatility behavior of the fluid, it is important to use information from the distillation curve when determining the composition of the surrogate so that the ultimate model is a more reliable representation of the thermophysical properties of the fluid.

Conclusions

In this paper, we presented a seven-component surrogate mixture model for the representation of the thermophysical

properties of synthetic aviation fuel S-8. A key feature in the development of the surrogate is the inclusion of experimental data from the advanced distillation curve metrology that permits improvements in the representation of the volatility behavior of the surrogate mixture. The procedure for correlating and incorporating the distillation curve data is general and may be applied to develop other surrogate fuel mixtures. Future work will use this process to determine surrogate models for complex fluids such as other aviation and rocket fuels, examples of which are RP-1, RP-2, and JP-8.

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