Thermodynamic, Transport, and Chemical Properties of “Reference” JP-8 (F1ATA06004G004)

Thomas J. Bruno
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Boulder, CO
National Institute of Standards and Technology

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NIST helps build the infrastructure for technological innovation.

We’re here to help you with problems related to measurement, standards, data, and technology.

...The Congress shall have Power To...

... and fix the Standard of Weights and Measures,
NIST Staff:

• Thomas J. Bruno, PI
• Marcia Huber
• Arno Laesecke
• Eric Lemmon
• Mark McLinden
• Stephanie L. Outcalt
• Richard Perkins
• Beverly L. Smith
Executive Summary:

AFOSR-MIPR F1ATA06004G004
(3/1/06)

• Characterization of a real fuel: JP-8
  – i.e., chemical analysis, \textbf{VLE}, \( \rho \), \( \nu \), \( \lambda \), \( C_v \),
• Standard reference measurement and modeling of fuel palette components.
• Develop a surrogate fluid model for real JP-8
• Relation to the synthetic JP-8 (Fischer Tropsch S-8 model)
• Solubility characterization of additive species
• We have examined:
  – 3 samples of Jet-A
  – 1 sample of a flightline JP-8
  – 1 sample of S-8
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• Related fluids:
  – 1 sample of CDF
  – 3 additional samples of FT fuels
  – 2 samples of bio-derived fuels
• We have examined:
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• Related fluids:
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While we must nail down $\rho$, $\nu$, $\lambda$, $C_v$, etc. to develop a model,

- The volatility of critical importance,

- n-decane: $\rho = 0.73$ g/mL
- n-hexadecane $\rho = 0.77$ g/mL

Granted, I’m hiding the temperature and pressure dependence, but there is not much difference with composition.
ADC:

• Practical way to measure VLE of complex fluids:
  – temperatures are true thermodynamic state points
  – consistent with a century of historical data
  – temperature, volume and pressure measurements of low uncertainty – EOS development
  – composition explicit data channel for qualitative, quantitative and trace analysis of fractions
  – energy content of each fraction
  – corrosivity of each fraction
  – greenhouse gas output of each fraction
  – thermal and oxidative stability of the fluids
Typical data suite for an aviation fuel:

ΔHc

Volume Fraction, %

Temperature, Tk, C

FTIR

SCD

MS

corrosivity
Compressed Liquid Density:
Compressed Liquid Densimeter

- Temperature range: –20 to 200°C

Pressure range: 0 MPa to 100 MPa

Density range: 0 – 3000 kg/m³
Three samples of Jet-A, and S-8:

\[ \rho l (\text{kg} \cdot \text{m}^3) \]

- Jet-A-3602
- Jet-A-3638
- Jet-A-4658
- S-8

Approved for public release; distribution unlimited.
Speed of sound data of jet fuels as a function of temperature at ambient pressure.
Adiabatic compressibility data of jet fuels as a function of temperature at ambient pressure.
Kinematic viscosity data of jet fuel JP-8 3773 flightline as a function of temperature at ambient pressure.
Temperature and Pressure Control
Thermal Conductivity of Jet A (4658)
Thermal Conductivity of JP-8

λ / W m⁻¹ K⁻¹

ρ / kg m⁻³

300 K
355 K
405 K
452 K
496 K
547 K

Approved for public release; distribution unlimited.
Now, to turn all of this into an Equation of State!
Why should Joe the Plumber care about equations of State?
## EOS Characteristics

<table>
<thead>
<tr>
<th></th>
<th>Vapor Phase</th>
<th>Liquid Phase</th>
<th>Critical region</th>
<th>Accuracy</th>
<th>Speed</th>
<th>Iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ideal gas law</td>
<td>√</td>
<td></td>
<td></td>
<td>Low</td>
<td>High</td>
<td>No</td>
</tr>
<tr>
<td>vdW</td>
<td>√</td>
<td>√</td>
<td>√</td>
<td>Low</td>
<td>High</td>
<td>No</td>
</tr>
<tr>
<td>Cubics</td>
<td>√</td>
<td>√</td>
<td>√</td>
<td>Moderate</td>
<td>High</td>
<td>No</td>
</tr>
<tr>
<td>Virials</td>
<td>√</td>
<td></td>
<td></td>
<td>Moderate</td>
<td>Med</td>
<td>Yes</td>
</tr>
<tr>
<td>BWRs</td>
<td>√</td>
<td>√</td>
<td>√</td>
<td>High</td>
<td>Med</td>
<td>Yes</td>
</tr>
<tr>
<td>Helmholtz</td>
<td>√</td>
<td>√</td>
<td>√</td>
<td>Very High</td>
<td>Low</td>
<td>Yes</td>
</tr>
</tbody>
</table>

All calculate pressure as a function of density and temperature, except for the Helmholtz energy.
All thermodynamic properties can be calculated as derivates from each of the four fundamental equations:

- Internal energy as a function of density and entropy
  - Entropy is not a measurable quantity.
- Enthalpy as a function of pressure and entropy
  - Cannot have a continuous equation across the phase boundary.
- Gibbs energy as a function of pressure and temperature
  - Cannot have a continuous equation across the phase boundary.
- Helmholtz energy as a function of temperature and density
  - Both temperature and density are measurable. Continuous across two-phase region.
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Given density and temperature, all other properties can be calculated

- Iterative solutions required given input conditions of pressure and temperature; pressure and enthalpy; pressure and entropy; saturation temperature; vapor pressure; etc.

\[ \frac{a(\rho, T)}{RT} = \alpha(\delta, \tau) = \alpha^0 + \alpha' \]
Properties calculated from an EOS

- Temperature
- Pressure
- Density
- Heat capacity
- Speed of sound
- Energy
- Entropy
- Enthalpy
- Fugacity
- Second virial coefficient
- Joule-Thomson coefficient

- Volume expansivity
- Compressibility
- Vapor-liquid equilibrium

*** Cannot calculate viscosity and thermal conductivity ***
REFPROP program

- www.nist.gov/srd/nist23.htm
- 90 pure fluids
- Mixtures with up to 20 components
- All thermodynamic and transport properties
- Table and plot generation
- Fluid search menu
# Thermal Conductivity of Jet A (4658)

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Conductivity</th>
<th>Chamber 1</th>
<th>Chamber 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 K</td>
<td>0.83098</td>
<td>14433.8</td>
<td>85.762</td>
</tr>
<tr>
<td>320 K</td>
<td>0.91735</td>
<td>14400.8</td>
<td>84.602</td>
</tr>
<tr>
<td>340 K</td>
<td>1.0043</td>
<td>14366.6</td>
<td>84.082</td>
</tr>
<tr>
<td>360 K</td>
<td>1.0823</td>
<td>14333.3</td>
<td>83.334</td>
</tr>
</tbody>
</table>

# Three samples of Jet-A, and S-8:

- **Jet-A 4658**
- **S-8**

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### Kinematic Viscosity Data of Jet Fuel JP-8 3773

- **f** as a function of temperature at ambient pressure.

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### FPROP

- **Dynamic and Transport Properties**
  - **Base 23**, Version 8.1beta, July 09, 2007
  - J. Huber, and M.O. McLinden
  - NIST's Chemical Properties Division
  - Secretary of Commerce on behalf of the United States of America. All Rights Reserved.

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### Speed of sound data of jet fuels as a function of temperature at ambient pressure.
• In prior years, we would start with density, then add fits to the other properties

• Now, we start with a chemical analysis, then the volatility (ADC), then add density and the rest of the mix
So, what if I ignore the volatility (i.e., the distillation curve)?

Volatility of S-8

- Experimental data, Bruno 2006
- 7 component surrogate, Huber et al 2008
- 10 component surrogate, Bruno 2006
And predictively, for JP-900
## The Surrogate Mixtures:

<table>
<thead>
<tr>
<th>Fluid Name</th>
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<th>Jet-A-3638, mole fraction</th>
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<tbody>
<tr>
<td>propylcyclohexane</td>
<td>0.000</td>
<td>0.009</td>
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<tr>
<td>hexylcyclohexane</td>
<td>0.000</td>
<td>0.275</td>
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<td>0.255</td>
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<td>0.014</td>
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<td>5-methylnonane</td>
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<td>2-methyldecane</td>
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<td>n-tetradecane</td>
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<td>0.027</td>
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Approved for public release; distribution unlimited.
So how did we do?
Density:

Samples differ by 1.5 %

Fit is to 0.1 %

$p=83$ kPa
Speed of Sound:

Samples differ by 3.5%

We overpredict by 1 - 3%

Jet A-3638 model
Jet A-4658 model

p=83 kPa
Viscosity:

Samples differ by 20%

Fit is to 3%

Jet A-3638
Jet A-4658
3638 model
4658 model

$\rho$-83 kPa

Temperature, K

Viscosity, $\mu$Pa.s

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Thermal Conductivity:

\[ 100\% \left( \frac{k_{\text{calc}} - k_{\text{exp}}}{k_{\text{exp}}} \right) \]

Fits are 0 – 4 %
Volatile (ADC):

Samples differ by up to 30 °C

Fit is to 0.2 °C

Jet A-3638
Jet A-4658
3638 model
4658 model

p=83 kPa
Conclusions:

• For most properties, the surrogate models for the “reference JP-8 (Jet-A) represent measurements to experimental uncertainty
Conclusions:

• For most properties, the surrogate models for the “reference JP-8 (Jet-A) represent measurements to experimental uncertainty

• When we are outside of experimental uncertainty, the models are as close as any we have done for complex fluids
But, in some ways, we generate even more questions:

– The “reference” Jet-A is 4658, an extremum in all properties

Recall the ADC measurements:
Recall, the energy content difference:
• The specs of Jet-A, JP-8 are so wide, we need a separate model for each sample

or,

• we need a composition-tunable model, the “dial” for which must be an easily measured property
• We are working on such an approach for RP-1, where the variability is:
  – probably not as large
  – but, currently not nailed down

• Such a follow-on effort will likely be needed for JP-8
Documentation:


More Documentation:


• Conspicuous by its absence is a paper on the thermodynamic model for JP-8.

• The fuel community should consider this unfinished business.
Acknowledgements

• AFOSR
  – Julian Tishkoff and Ralph Anthenien

• Tim Edwards, AFRL