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

Thomas J. Bruno
Physical and Chemical Properties Division
National Institute of Standards and Technology
Boulder, CO
NIST Boulder Laboratories

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NIST Staff:

- Tom Bruno
- Arno Laesecke
- Stephanie Outcalt
- Richard Perkins
- Marcia Huber
- Eric Lemmon
- Jason Widegren
and Students:

• Beverly Smith
• Lisa Ott
• Kari Brumbeck
• Amelia Hadler
• Tara Lovestead
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
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.
Volatility, on the other hand, changes dramatically with composition:
Advanced Distillation Curve Method

Distillation Curve???

For a complex mixture, it is a plot of the distillation temperature against cut fraction

- T vs. Vol
- T vs. 100 mL Volume
- T vs. Volume %
  (sometimes expressed as % evaporated)
ADC:

- An extension of classical (ASTM D-86) methods:
  - 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
The basics.
The adapter, and the receiver.
Typical data suite for an aviation fuel:

- **FTIR**: Fourier Transform Infrared Spectroscopy
- **SCD**: Sulfur Content Determination
- **MS**: Mass Spectrometry
- **ΔHc**: Heat of combustion

![Graph showing temperature (Tk, °C) vs. volume fraction (%)](image)

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Compressed Liquid Density:
**Densimeter**

- Anton Paar* DMA-HPM Density Measuring Cell
- Tube material: Hastelloy C-276
- Temperature range: –20 to 200° C
  Pressure range: 0 MPa to 100 MPa
  Density range: 0 – 3000 kg/m³
- Combined overall uncertainty in density: 0.64 to 0.81 kg/m³

*No recommendation or endorsement by NIST is implied.
Thermostated Housing

- Copper pipe with heaters and cooling channels
- Pneumatic valves
- Pre-heat loop on inlet
- 3 PRTs
- Insulation packed inside of and surrounding pipe
Temperature Control

- Thin film and mica heaters
- Three heating zones
- Circulator for sub-ambient temperatures
- SPRT and two 100 Ω PRTs
- Independently run PID loop
- Long-term stability ± 5 mK
- Thermal switches to protect against over heating
Pressure Control

- Programmable Syringe Pump
- Pneumatic valves
- Oscillating quartz crystal pressure transmitter (thermostated to \(\approx 40^\circ C\))
- Rupture discs to prevent over pressurization
Three samples of Jet-A:
and with S-8:
and finally the flightline sample
Density and Speed of Sound
5 °C to 70 °C, uncertainty 0.1%

Viscosity
20 °C to 100 °C, uncertainty 1.5%

- commercial instruments
- scan $T$-range in 3 hours
- calibration with standard fluids required
- small sample volumes (5 mL)
- contamination possible

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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.
Thermal Conductivity Measurements on Fuels

- Transient Hot-Wire Apparatus at NIST
  - Vapor, liquid, and supercritical fluid phases
  - Temperature Range $30 \, \text{K} < T < 750 \, \text{K}$
  - Pressure Range $0.01 \, \text{MPa} < P < 70 \, \text{MPa}$
  - Less than 0.5% uncertainty for liquids below 450 K
  - Uncertainty increases at high temperatures due to thermal radiation and sample decomposition

- Summary of Measurements on Liquid Fuels
  - Isotherms measured from $300 \, \text{K}$ to $550 \, \text{K}$ with pressures to 60 MPa
  - Significant cracking observed at temperatures above 600 K
  - Accurate thermal conductivity data obtained from $300 \, \text{K}$ to $550 \, \text{K}$
  - Performance verified with argon gas and toluene liquid
Schematic of Hot-Wire Bridge

Diagram:

- Main Power Relay
- Dummy Load Resistance
- Power Supply
- +V/2
- −V/2
- R1
- R2
- R3
- R4
- Imbalance Voltage
- Hot-Wire Bridge
- Ground
- Cell Wall
- Long Hot Wire
- Short Hot Wire

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Hot-Wire Cell and Pressure Vessel
Temperature and Pressure Control
Hot-Wire Measurement
Electronics
Thermal Conductivity of Jet A (3602)

\[ \lambda / \text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \]

\[ P / \text{MPa} \]


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Thermal Conductivity of Jet A
(3638)
Thermal Conductivity of Jet A (4658)
Thermal Conductivity of JP-8
So why should I care about equations of state?
## EOS Characteristics

<table>
<thead>
<tr>
<th>EOS Type</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>
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<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.
Types of fundamental equations

All thermodynamic properties can be calculated as derivatives 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.
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
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
In the remaining 4 months:

- The necessary equations of state for the surrogates will be completed.
- The surrogate model will be completed.
- The RefProp fluid files will be completed.
- Reports and papers will be completed.
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