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

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National Institute of Standards and Technology

Boulder, CO

NIST Boulder Laboratories

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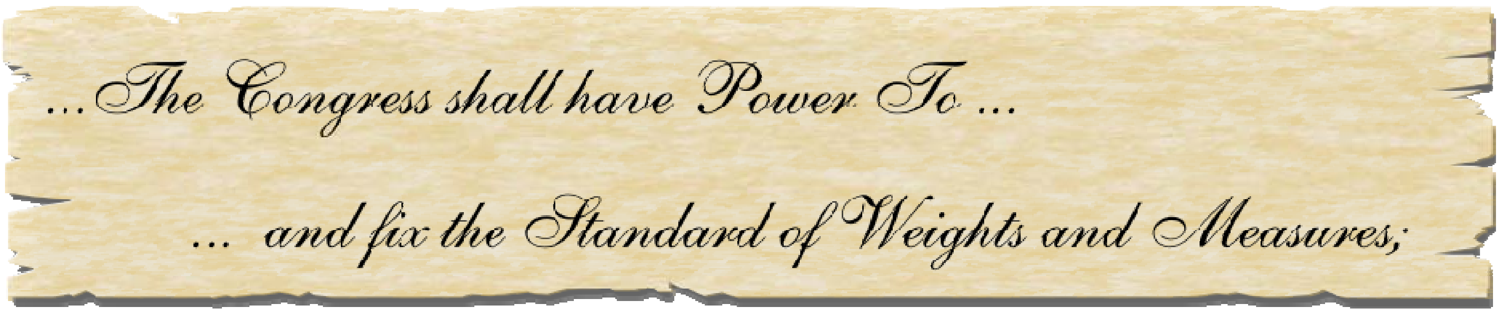

NIST Staff:

- 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, **VLE**, **ρ, υ, λ, 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

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While we must nail down ρ, υ, λ, C_v, etc. to develop a model,

- The volatility of critical importance,

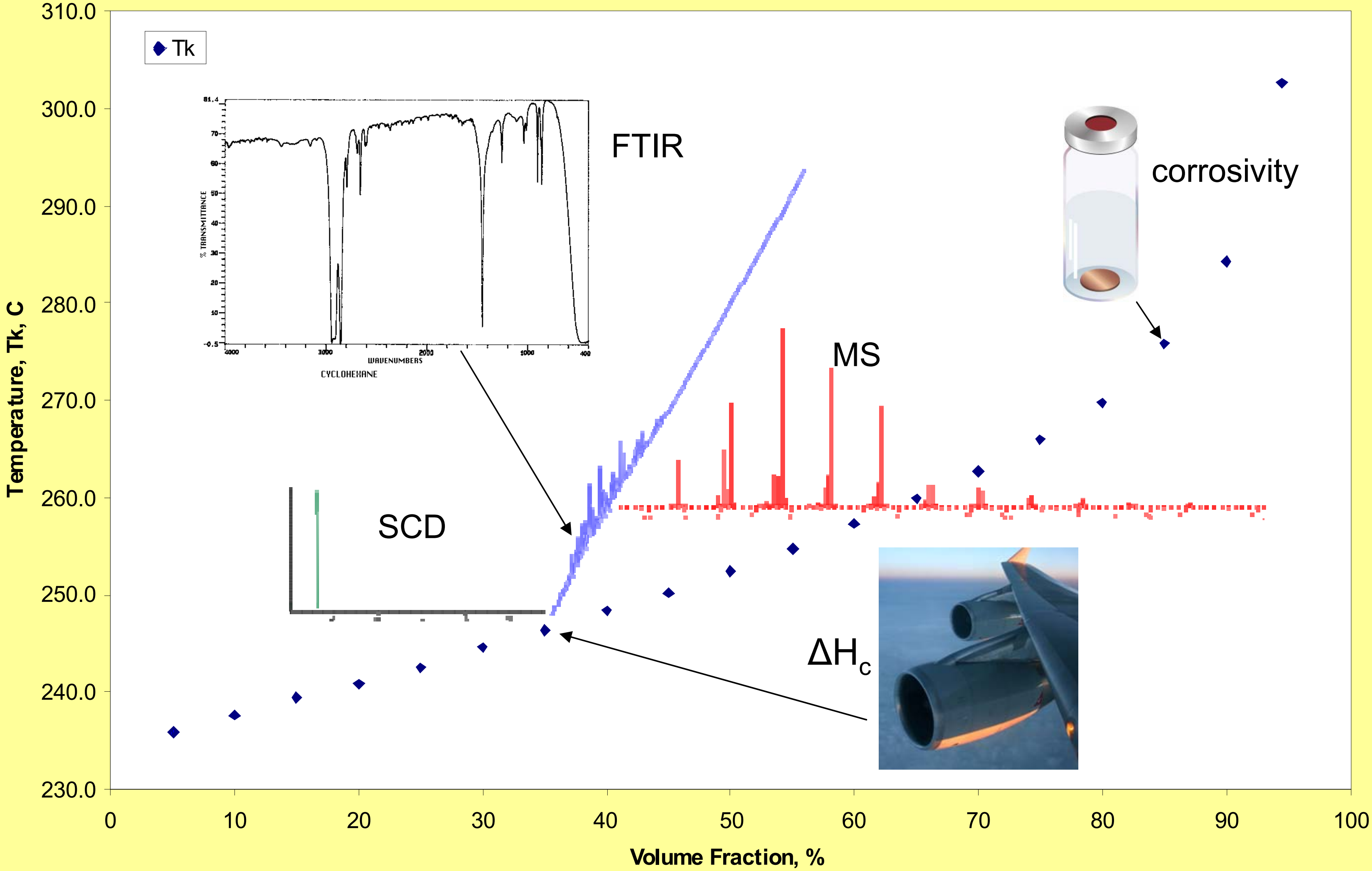
- n-decane: $\rho = 0.73$ g/mL
- n-hexadecane $\rho = 0.77$ g/mL

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:



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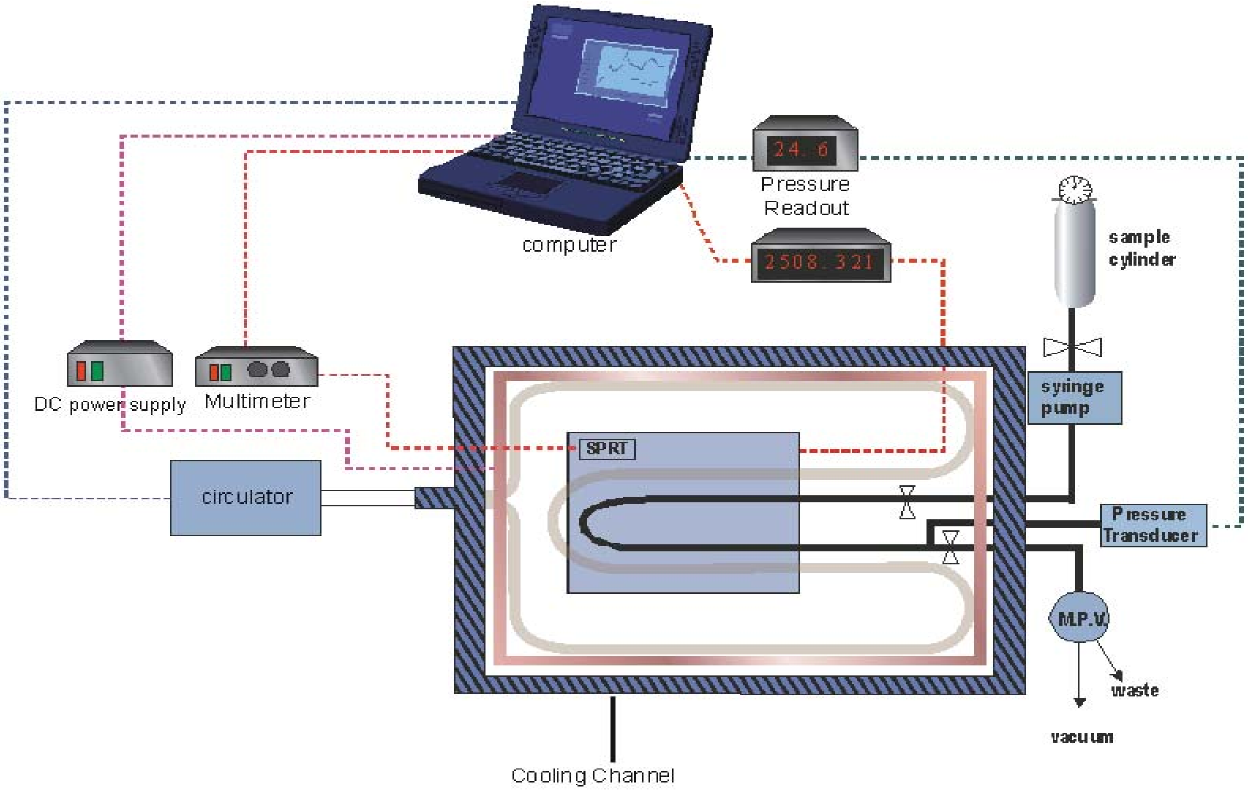
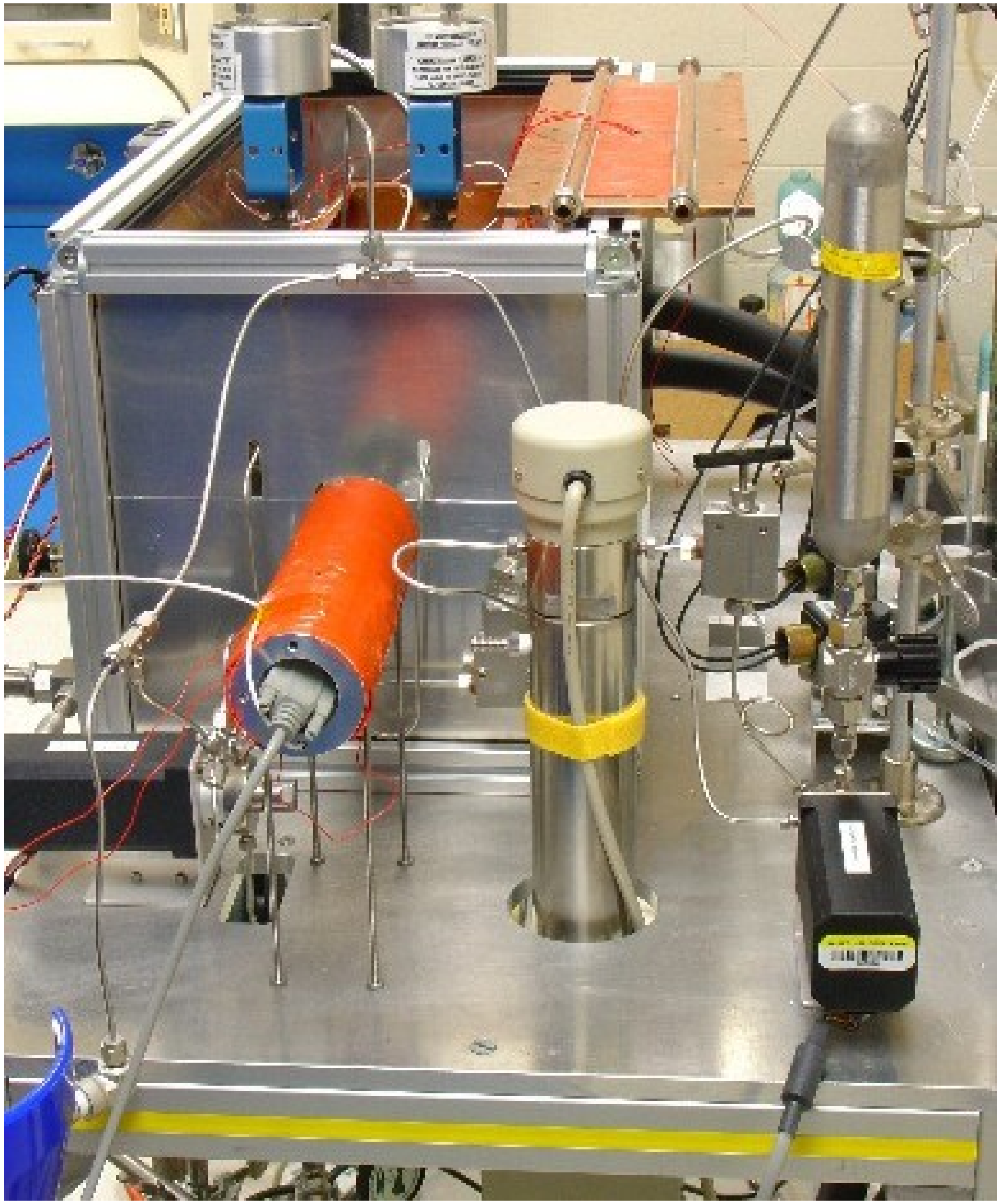
Compressed Liquid Density:



Compressed Liquid Densimeter

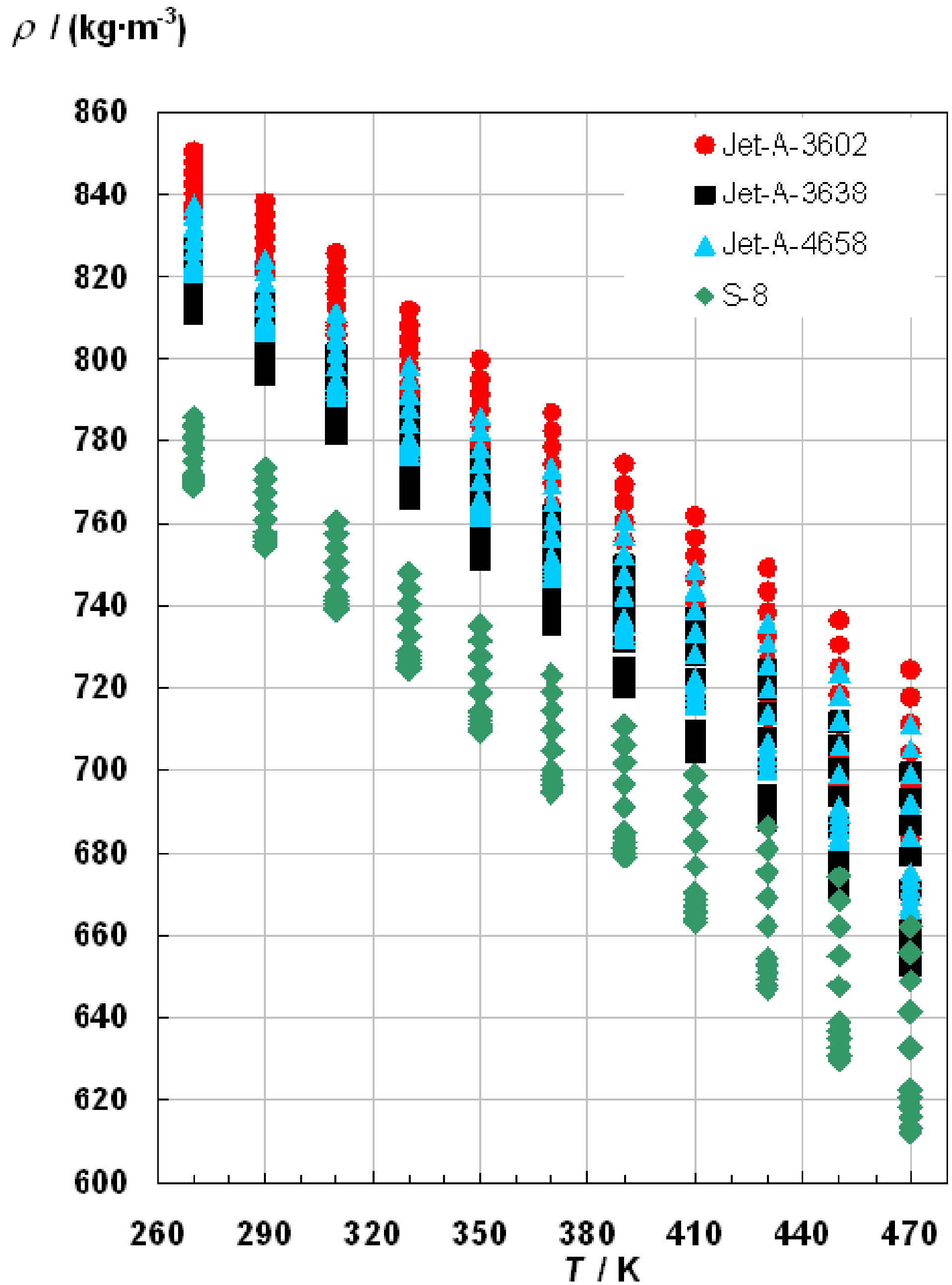


- Temperature range: –20 to 200° C

  Pressure range: 0 MPa to 100 MPa

  Density range: 0 – 3000 kg/m3

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



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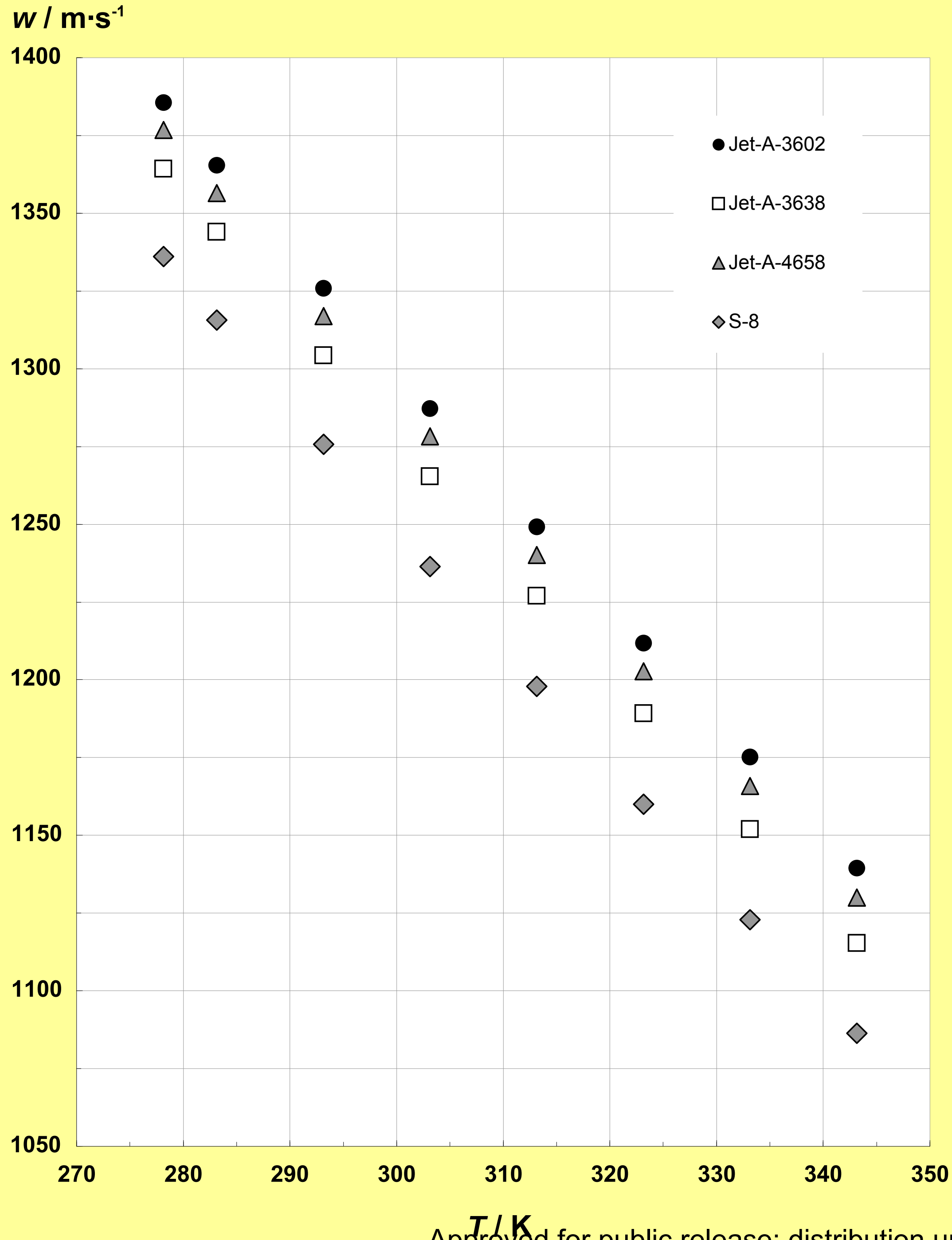
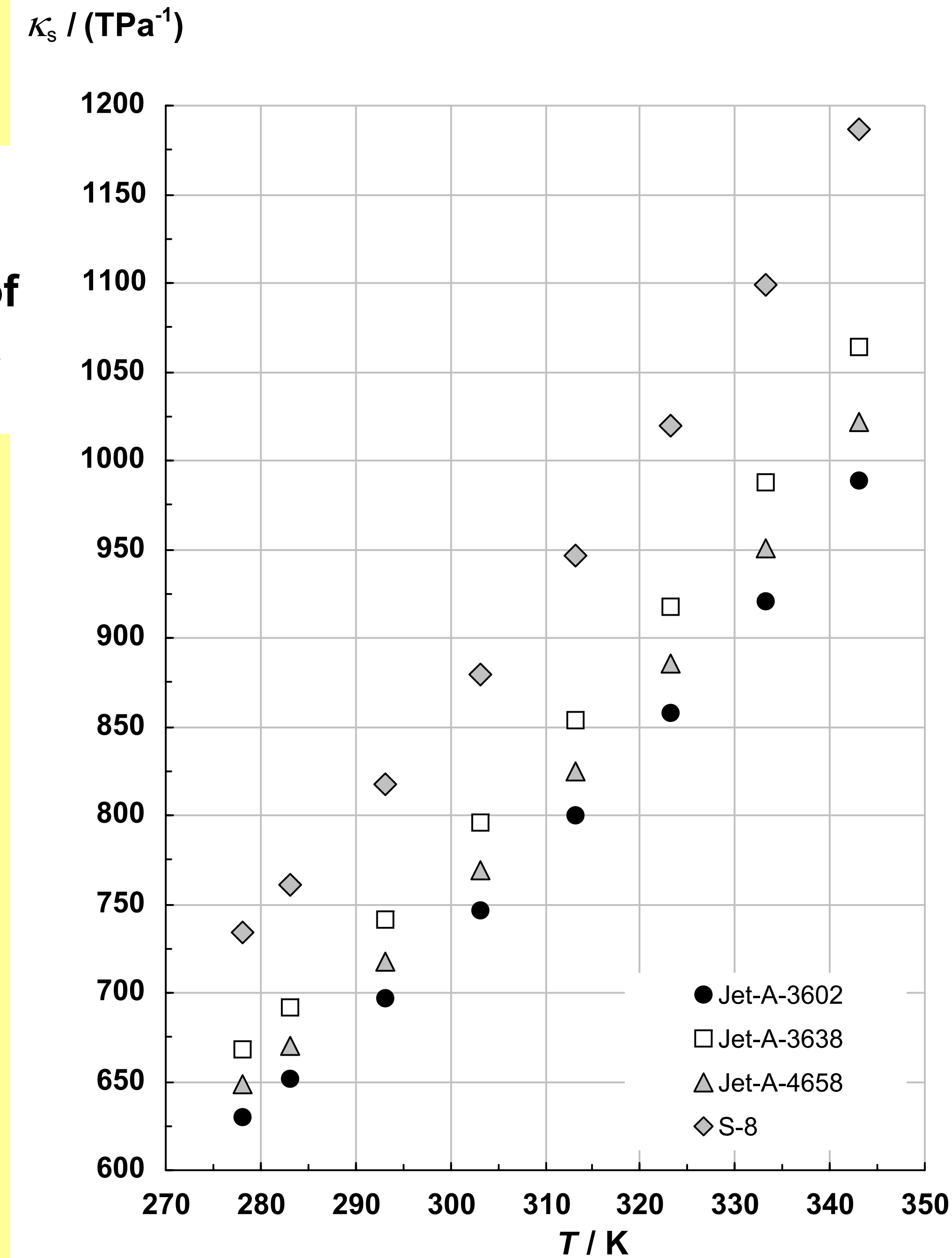
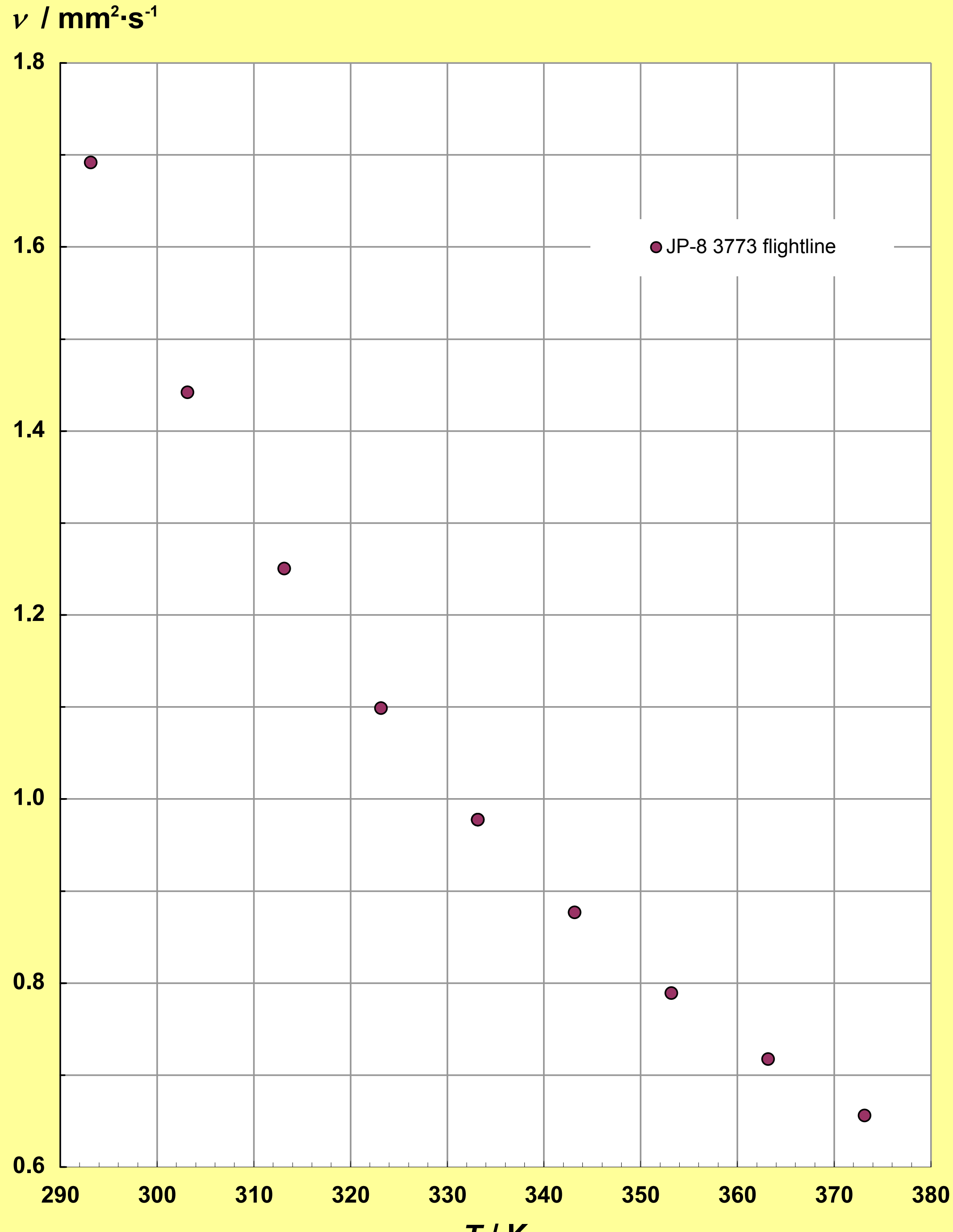
Speed of sound data of jet fuels as a function of temperature at ambient pressure.



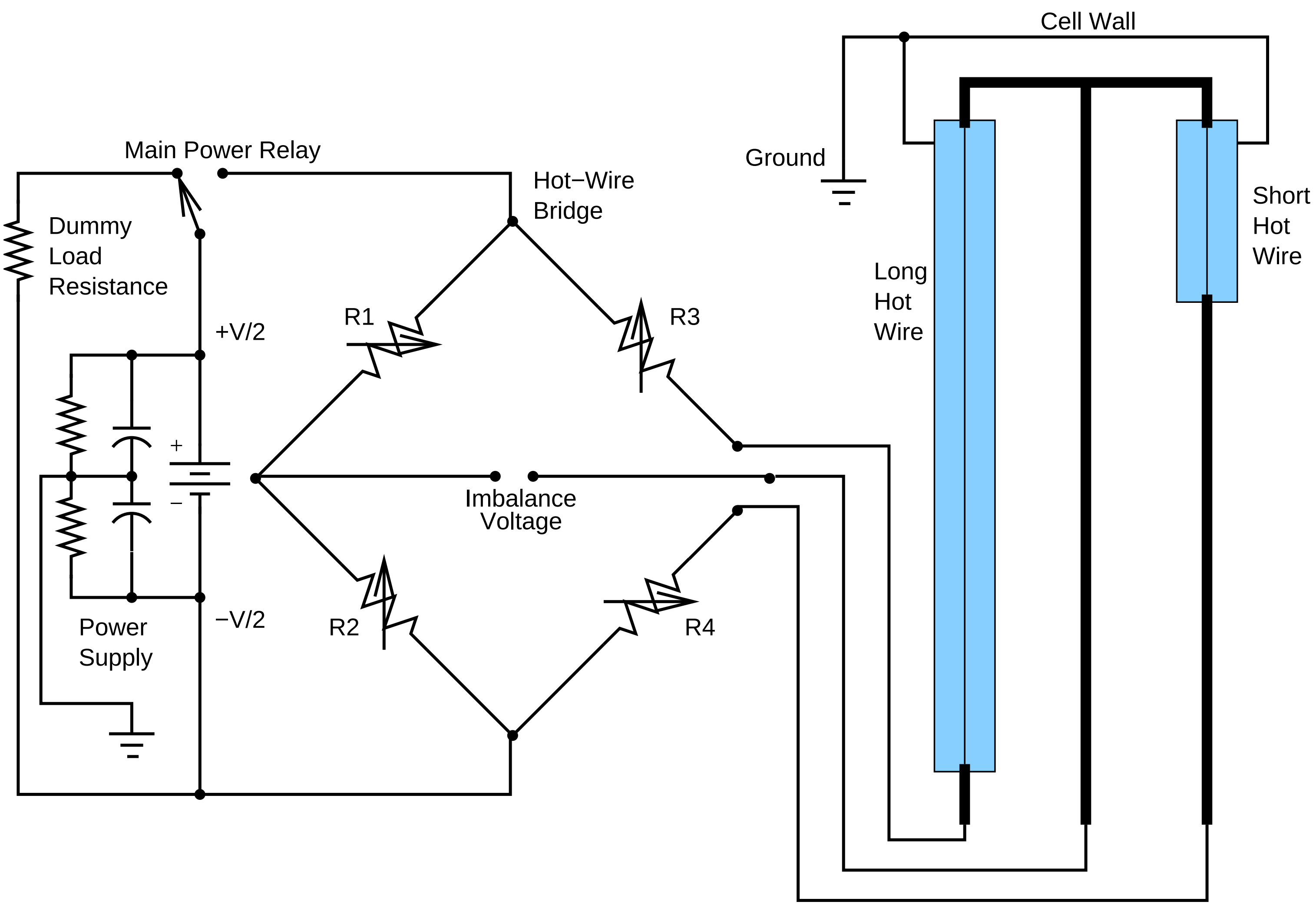
Adiabatic compressibility data of jet fuels as a function of temperature at ambient pressure.



Kinematic viscosity data of jet fuel JP-8 3773 flightline as a function of temperature at ambient pressure.

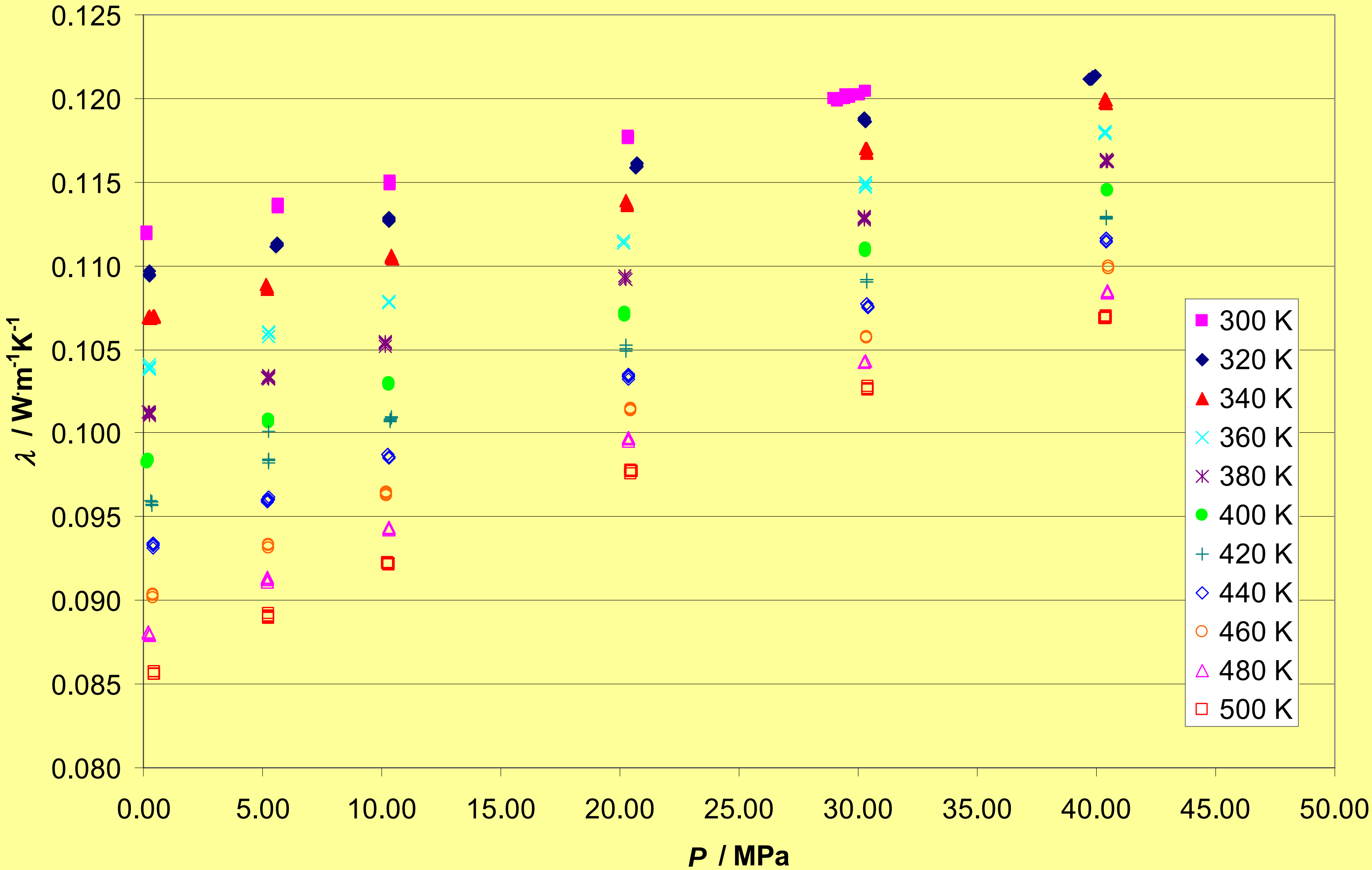


Hot Wire Thermal Conductivity Apparatus



Temperature and Pressure Control

Thermal Conductivity of Jet A (4658)



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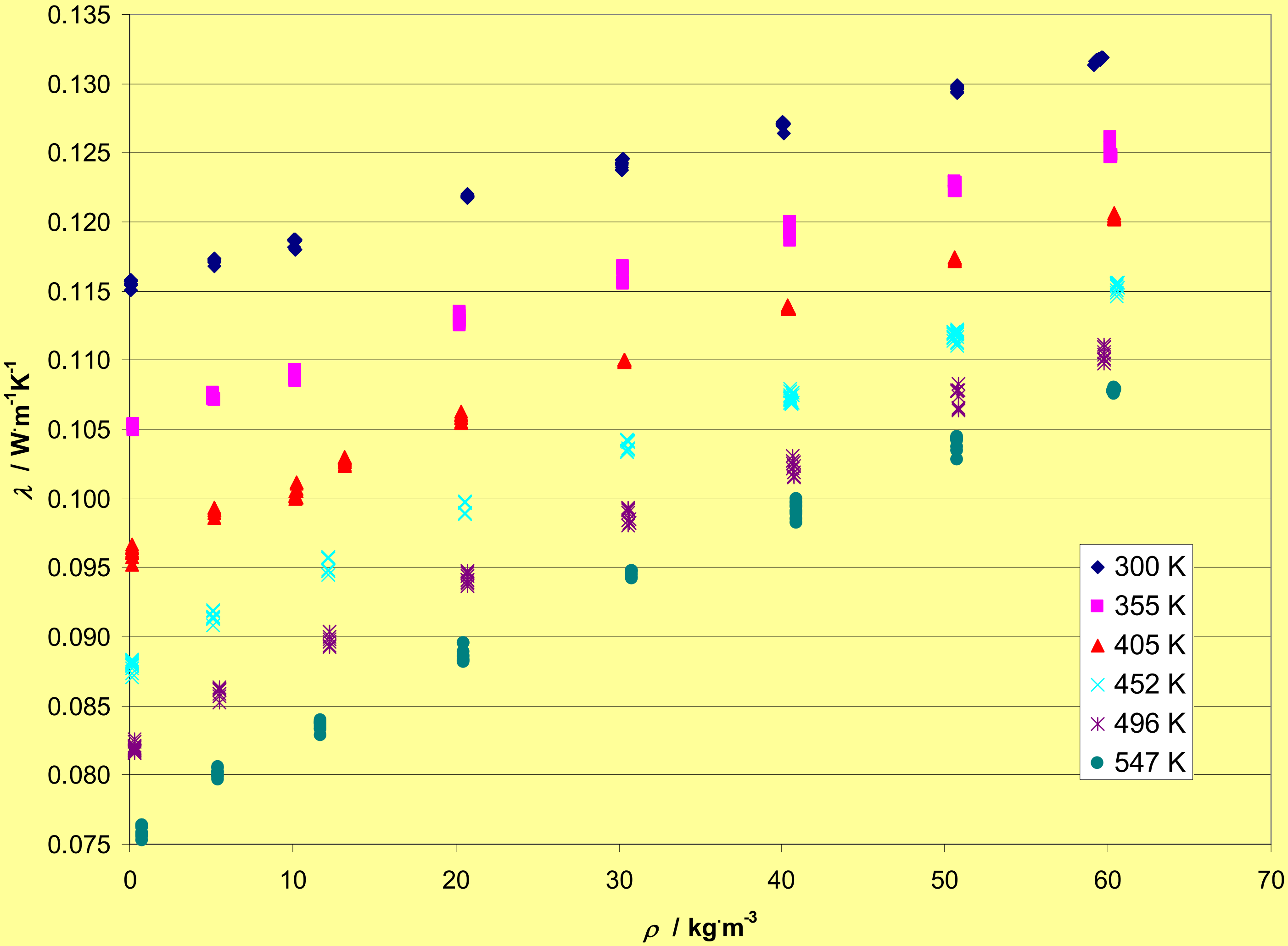
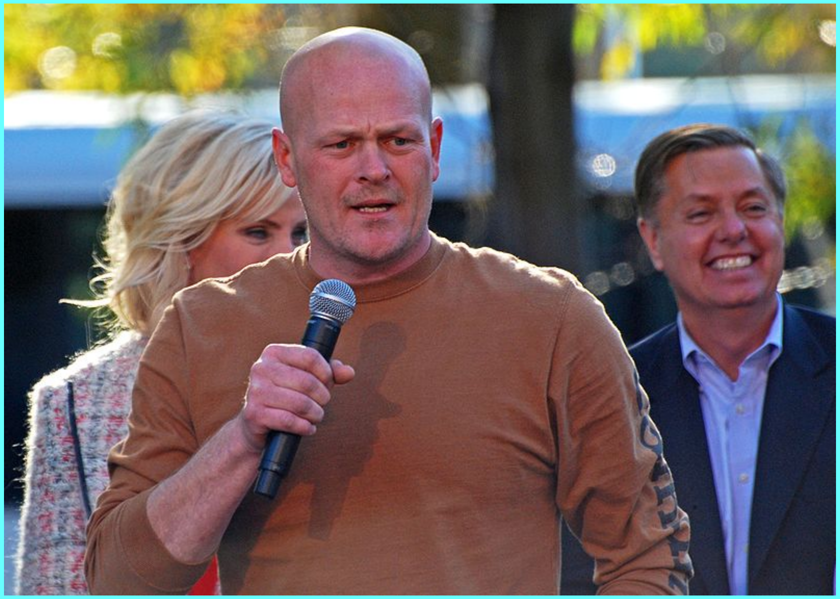
Thermal Conductivity of JP-8



Now, to turn all of this into an Equation of State!

Why should Joe the Plumber care about



equations of State?


USA
NASA
E85 / Gasoline

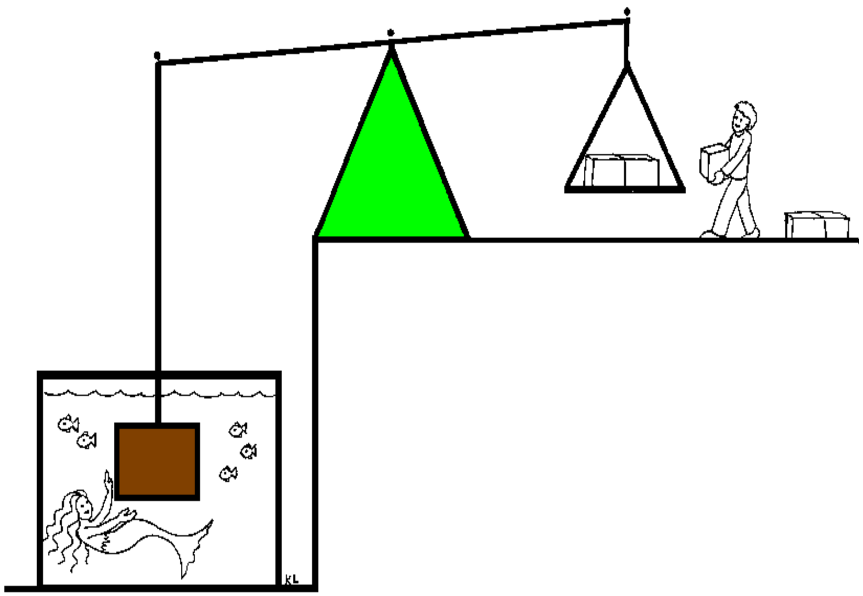
EOS Characteristics

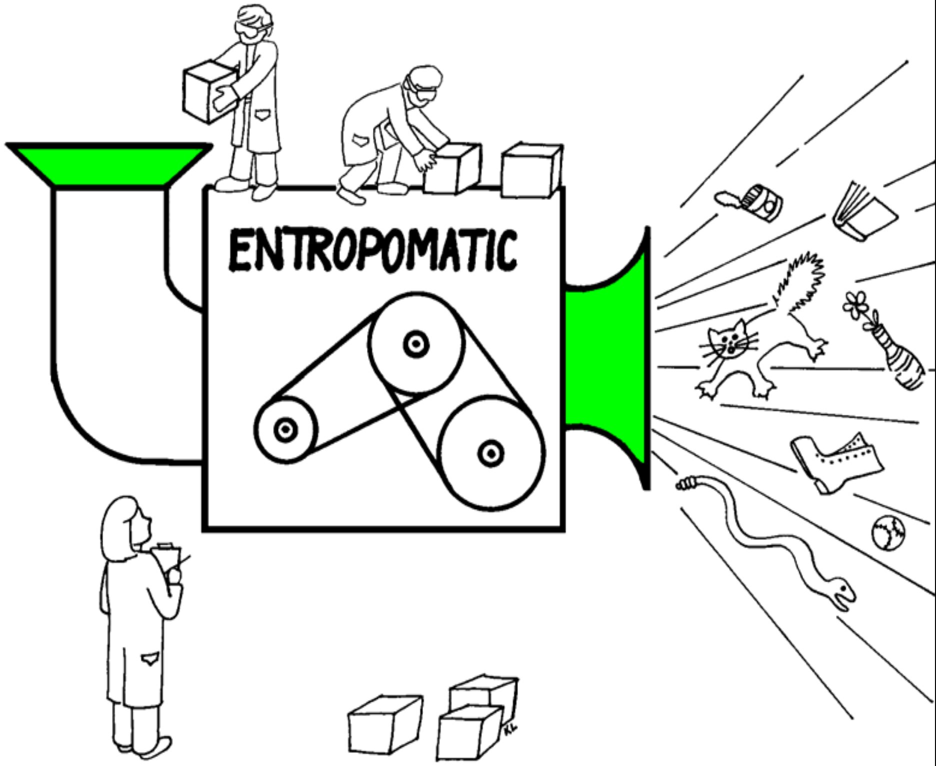
	Vapor Phase	Liquid Phase	Critical region	Accuracy	Speed	Iteration
Ideal gas law	√			Low	High	No
vdW	√	√	√	Low	High	No
Cubics	√	√	√	Moderate	High	No
Virials	√			Moderate	Med	Yes
BWRs	√	√	√	High	Med	Yes
Helmholtz	√	√	√	Very High	Low	Yes
All calculate pressure as a function of density and temperature, except for the Helmholtz energy						

Types of fundamental equations

All thermodynamic properties can be calculated as derivates from each of the four fundamental equations:

- Internal energy as a function of density and entropy
  - Entropy is not a measurable quantity.

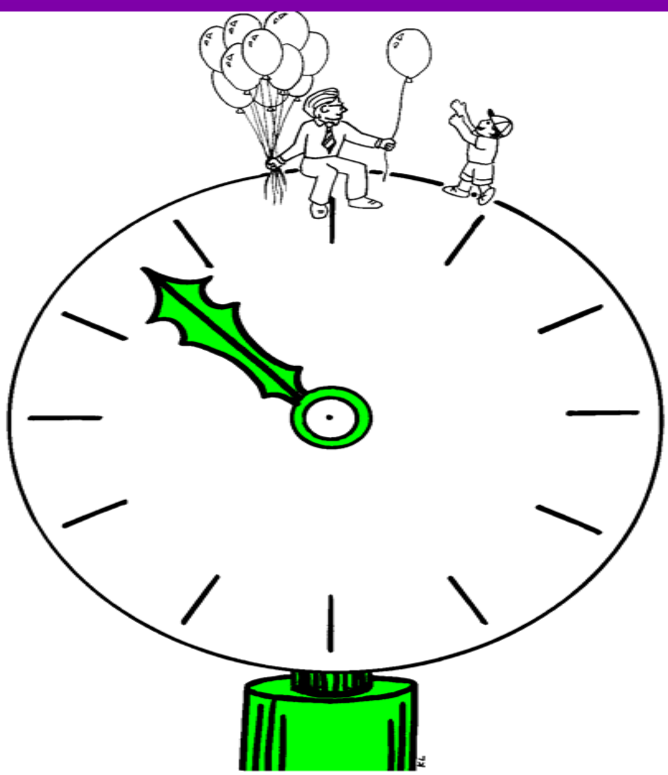


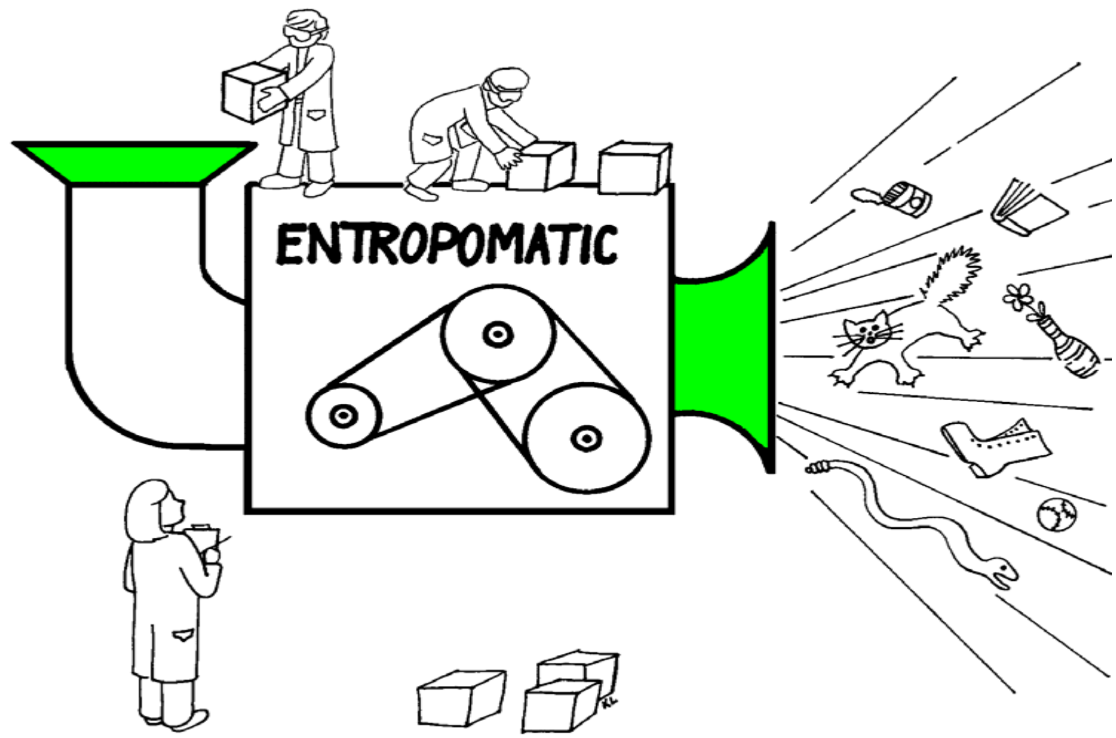


Types of fundamental equations

All thermodynamic properties can be calculated as derivates from each of the four fundamental equations:

- Enthalpy as a function of pressure and entropy
  - Entropy is not a measurable quantity. Cannot have a continuous equation across the phase boundary.

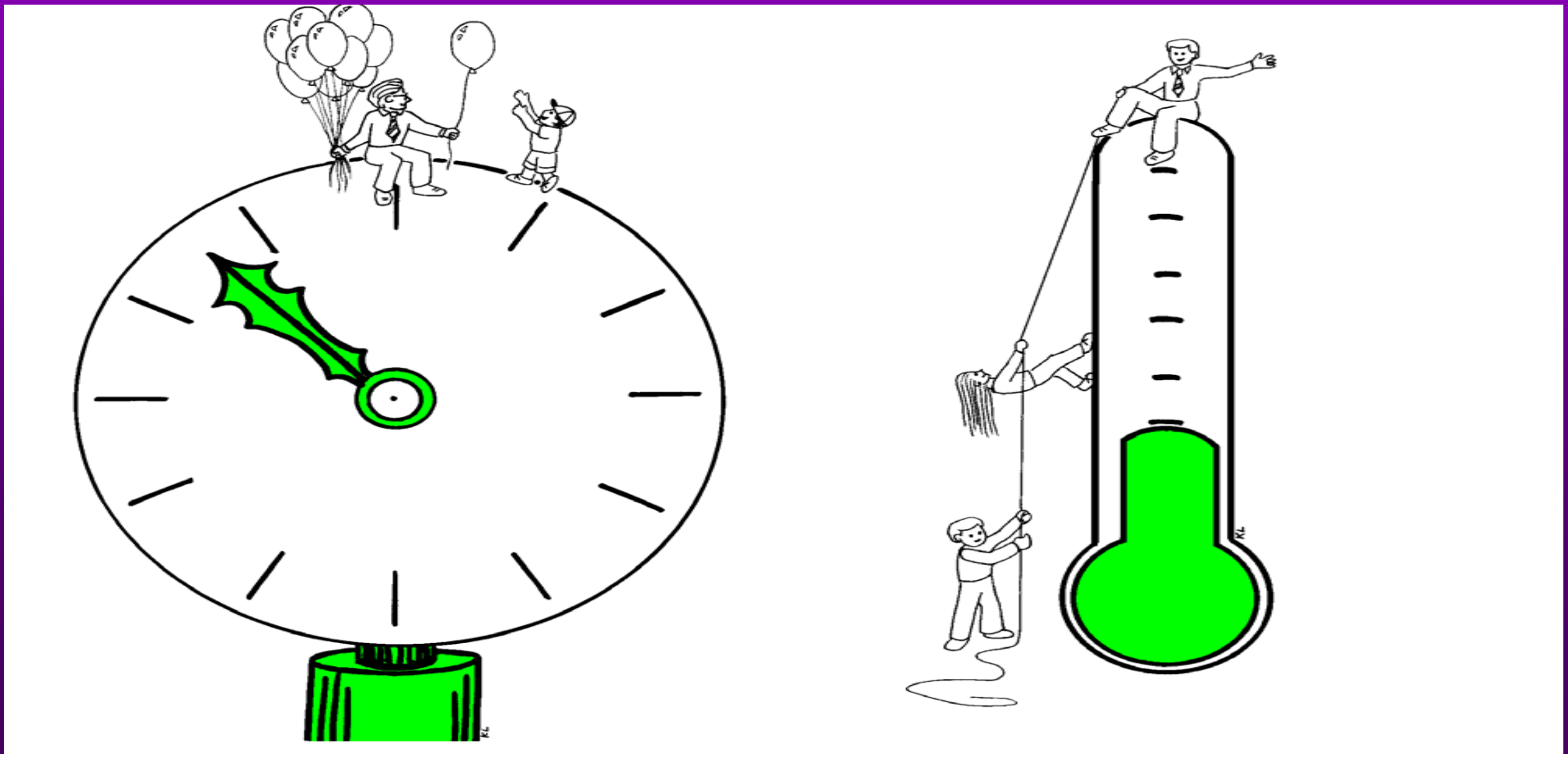




Types of fundamental equations

All thermodynamic properties can be calculated as derivates from each of the four fundamental equations:

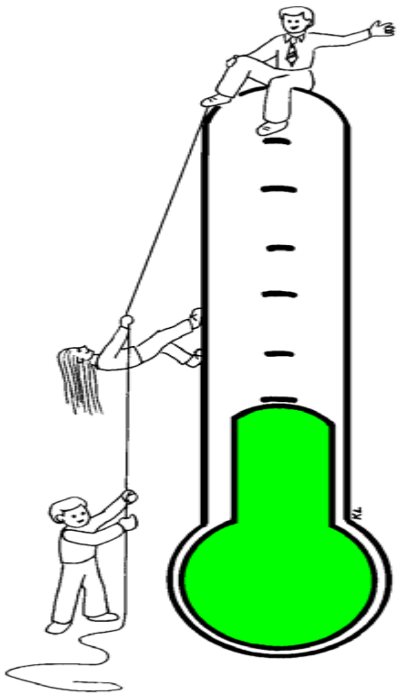
- Gibbs energy as a function of pressure and temperature
  - Cannot have a continuous equation across the phase boundary.

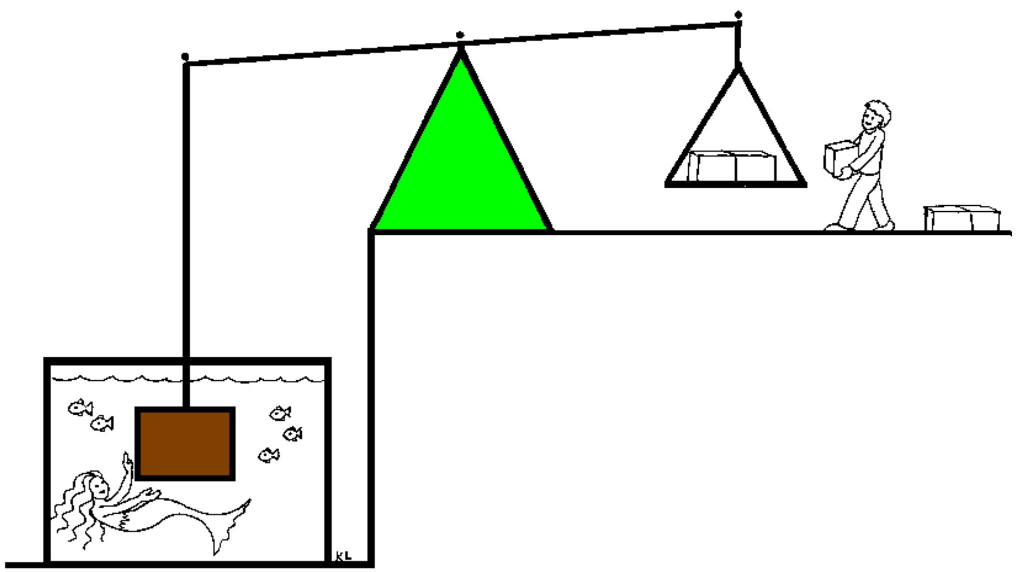


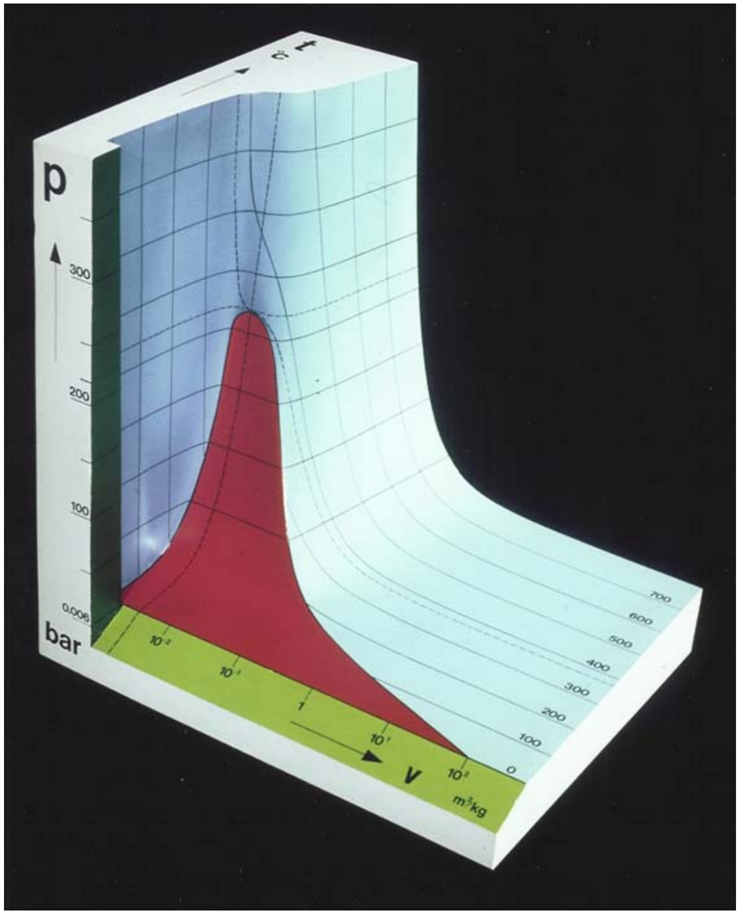
Types of fundamental equations

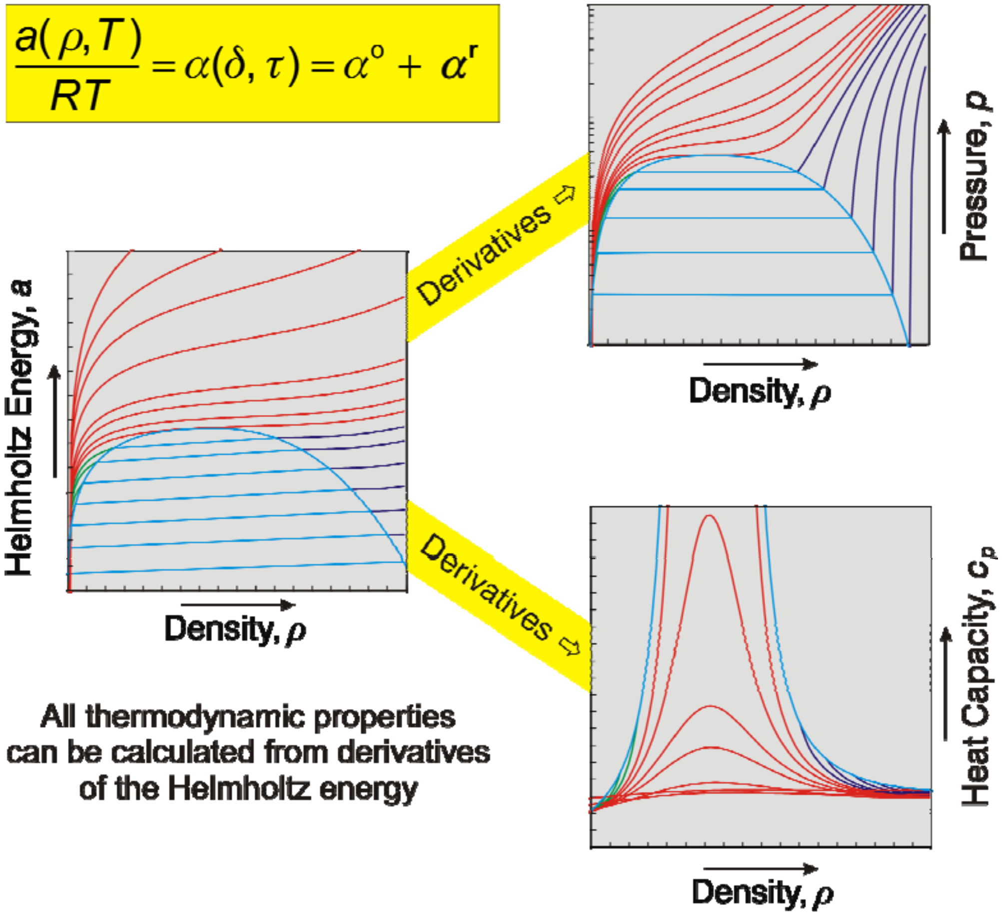
All thermodynamic properties can be calculated as derivates from each of the four fundamental equations:

- Helmholtz energy as a function of temperature and density
  - Both temperature and density are measurable. Continuous across two-phase region.









- 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.

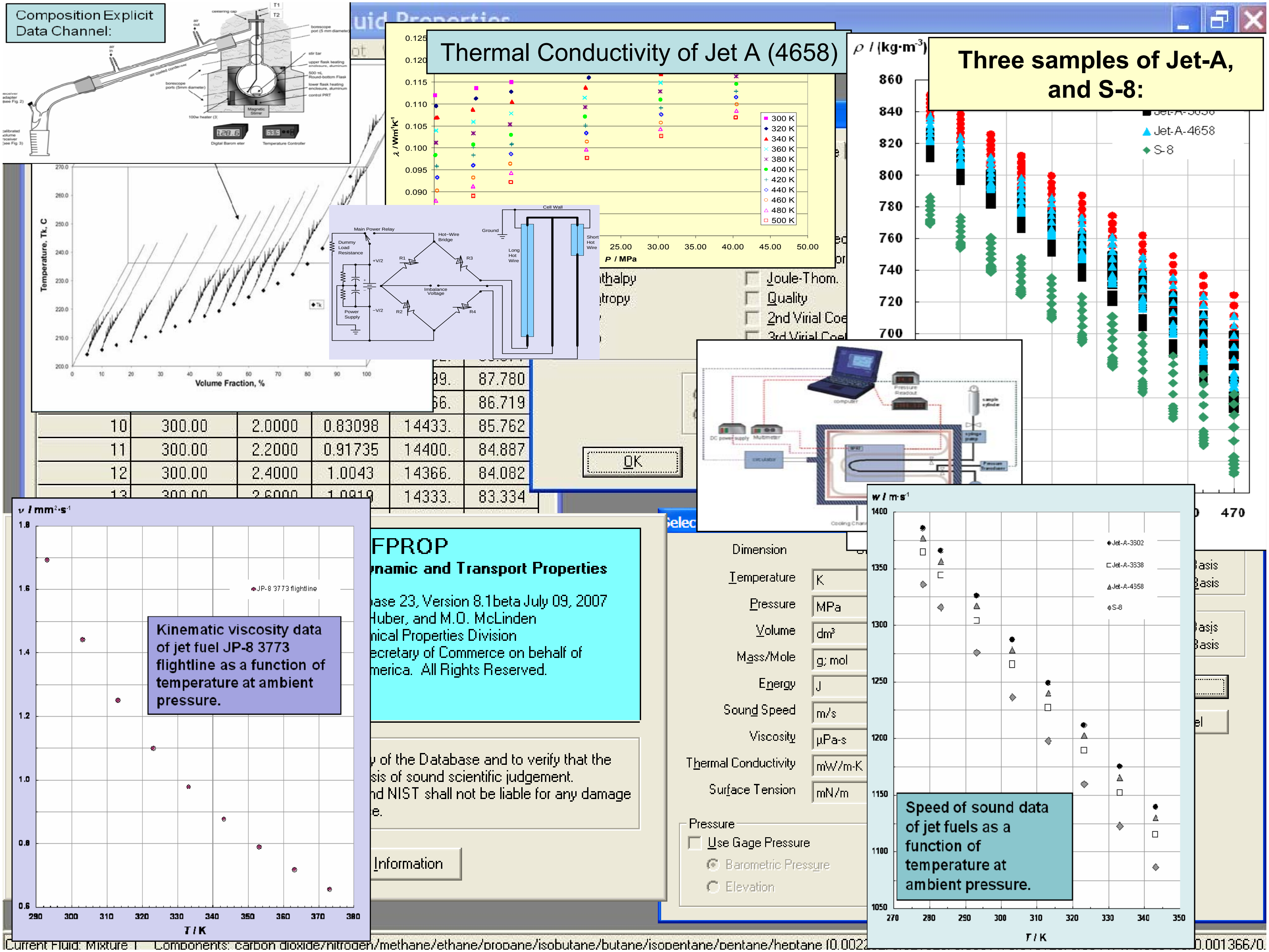
Properties calculated from an EOS

- 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

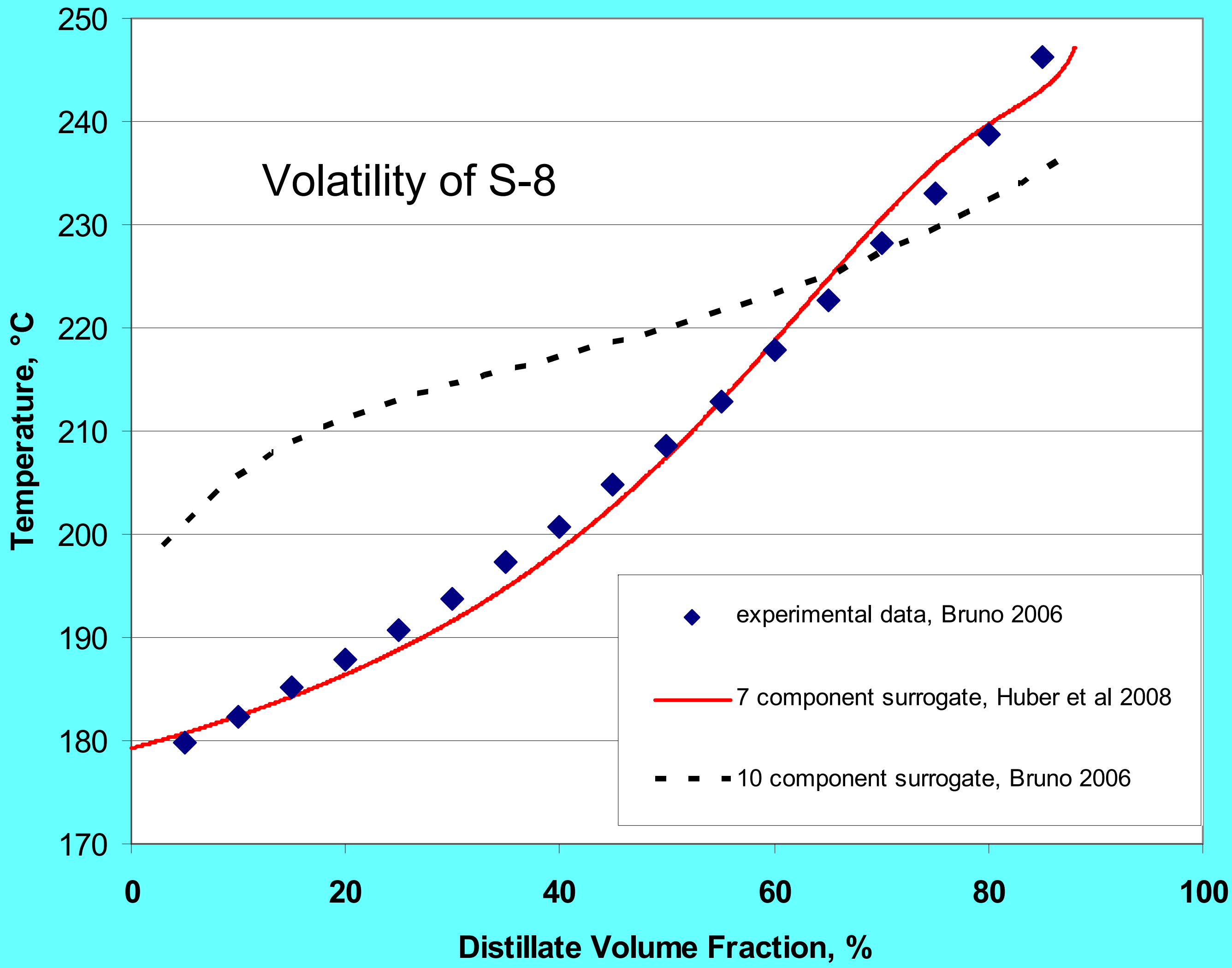
- www.nist.gov/srd/nist23.htm
- 90 pure fluids
- Mixtures with up to 20 components
- All thermodynamic and transport properties
- Table and plot generation
- Fluid search menu


Composition Explicit Data Channel:
Thermal Conductivity of Jet A (4658)
Three samples of Jet-A, and S-8:
Jet-A-4658
S-8
Kinematic viscosity data of jet fuel JP-8 3773 flightline as a function of temperature at ambient pressure.
Speed of sound data of jet fuels as a function of temperature at ambient pressure.
Volume Fraction, %
Temperature, Tk, C
Main Power Relay
Hot-Wire Bridge
Imbalance Voltage
Cell Wall
Long Hot Wire
Short Hot Wire
FPROP
Thermodynamic and Transport Properties
base 23, Version 8.1beta July 09, 2007
Huber, and M.O. McLinden
Information
Dimension
Temperature K
Pressure MPa
Volume dm³
Mass/Mole g; mol
Energy J
Sound Speed m/s
Viscosity μPa-s
Thermal Conductivity mW/m-K
Surface Tension mN/m
Use Gage Pressure
Barometric Pressure
Elevation
Joule-Thom.
Quality
2nd Virial Coe
OK
Current Fluid: Mixture
Components: carbon dioxide/nitrogen/methane/ethane/propane/isobutane/butane/isopentane/pentane/heptane

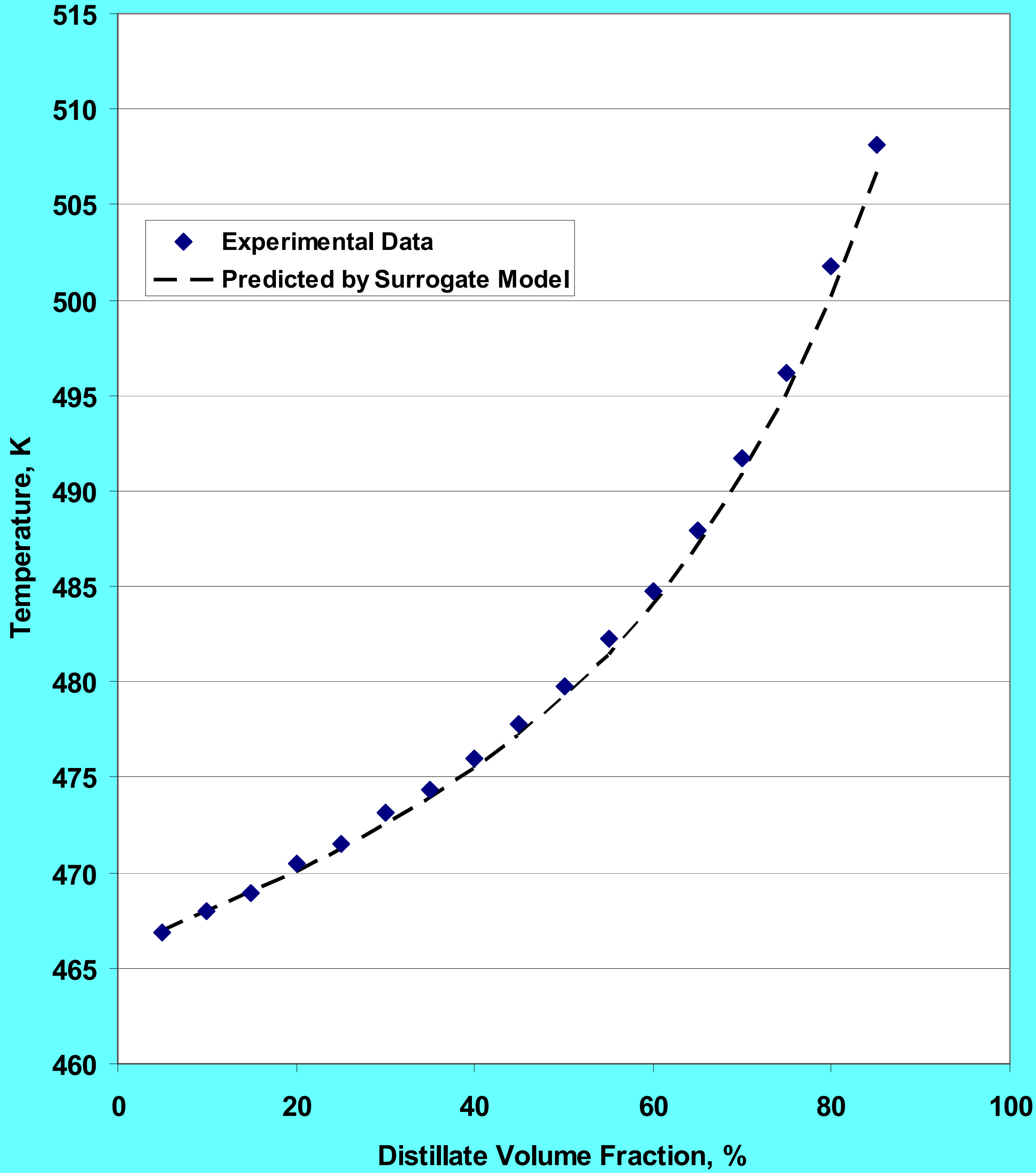
- In prior years, we would start with density, then add fits to the other properties

- 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)?



And predictively, for JP-900



The Surrogate Mixtures:

Fluid Name	Jet-A-4658, mole fraction	Jet-A-3638, mole fraction
propylcylcohexane	0.000	0.009
hexylcyclohexane	0.000	0.275
heptylcyclohexane	0.255	0.000
methyldecalin	0.081	0.014
5-methylnonane	0.148	0.068
2-methyldecane	0.164	0.347
n-tetradecane	0.068	0.027
n-hecadecane	0.030	0.000
ortho-xylene	0.055	0.120
tetralin	0.199	0.140

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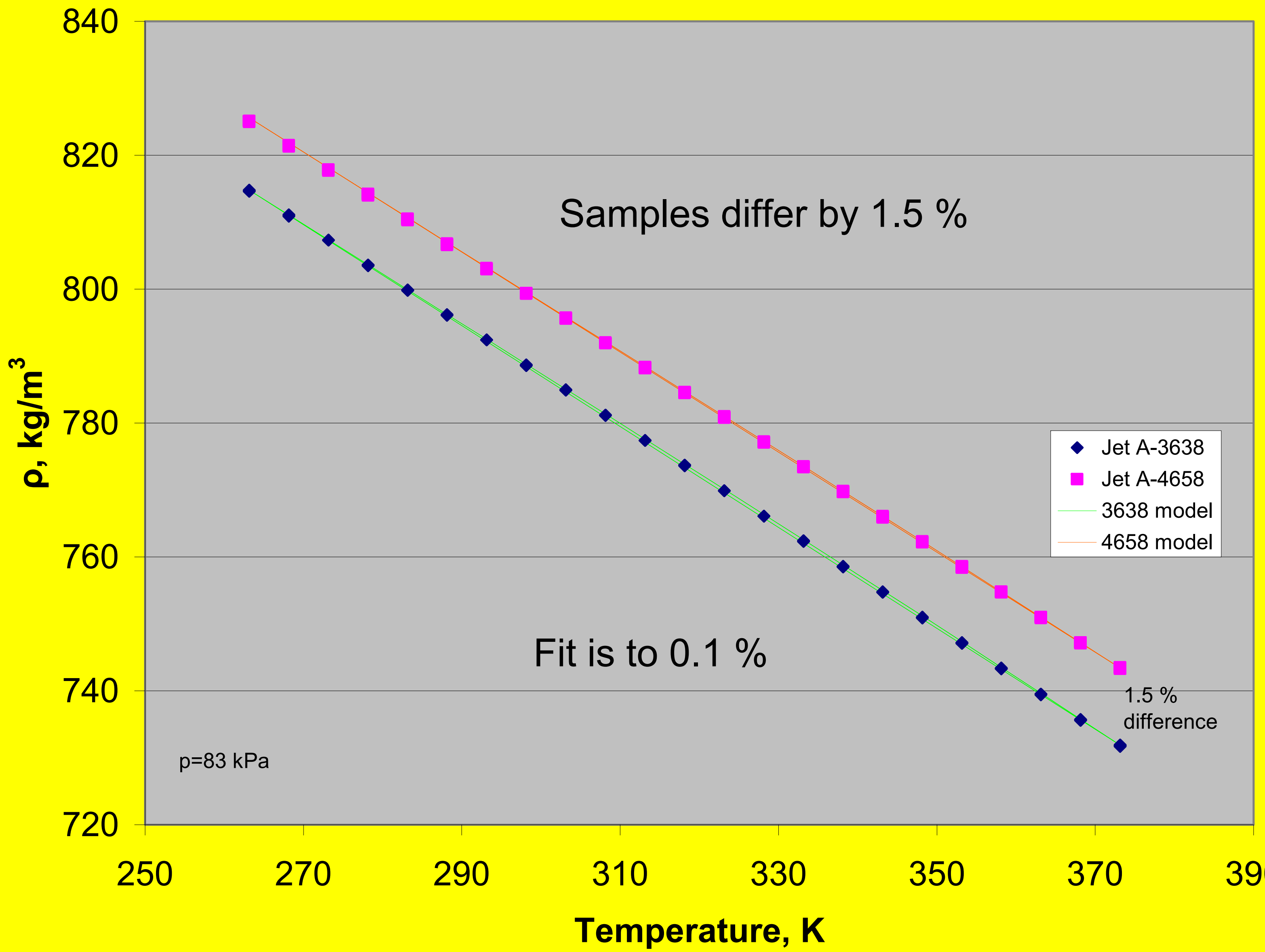
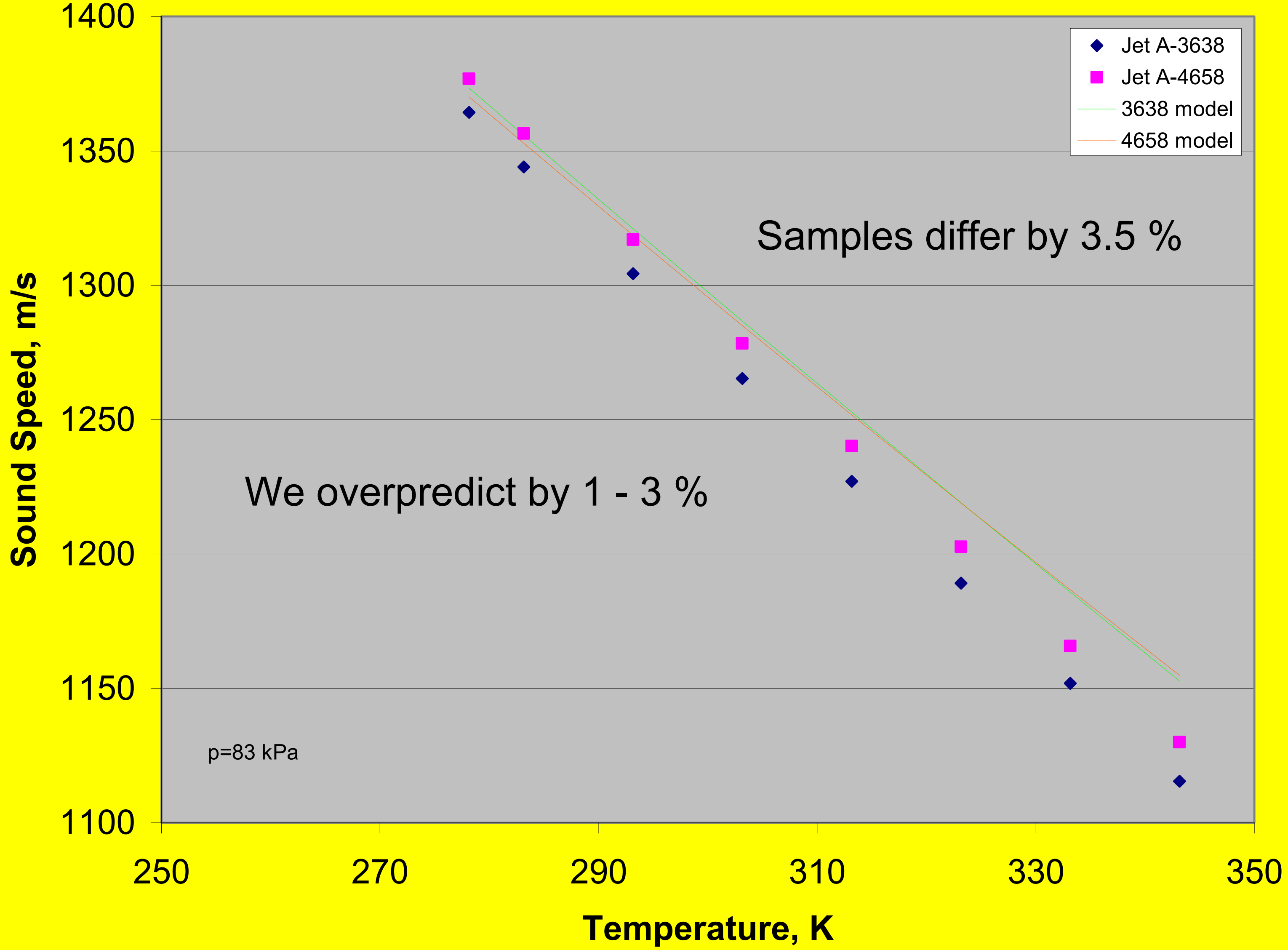
So how did we do?

Density:

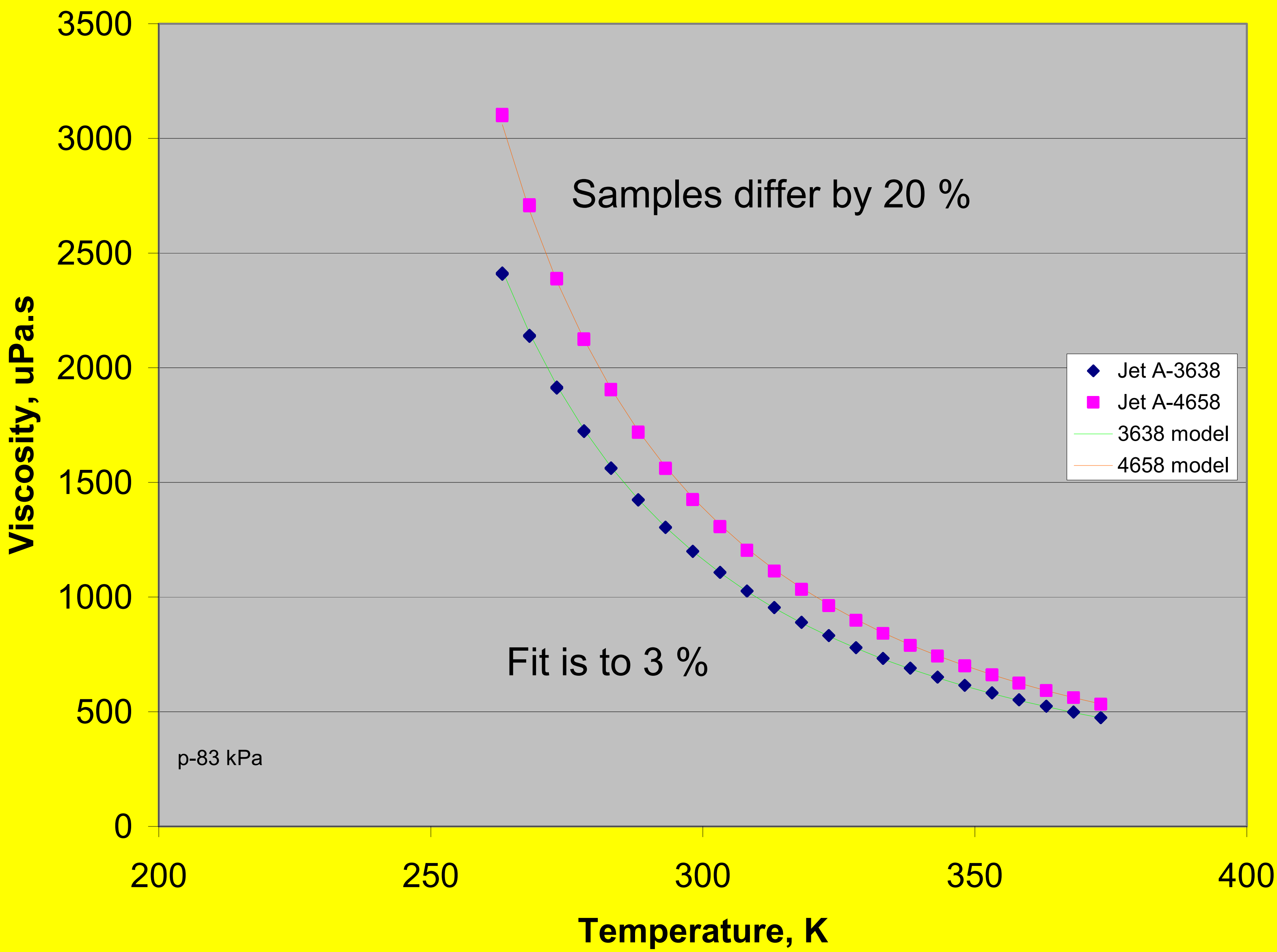


840
820
800
780
760
740
720
250
270
290
310
330
350
370
390
ρ, kg/m³
Temperature, K
Samples differ by 1.5 %
Fit is to 0.1 %
Jet A-3638
Jet A-4658
3638 model
4658 model
1.5 %
difference
p=83 kPa

Speed of Sound:



Viscosity:



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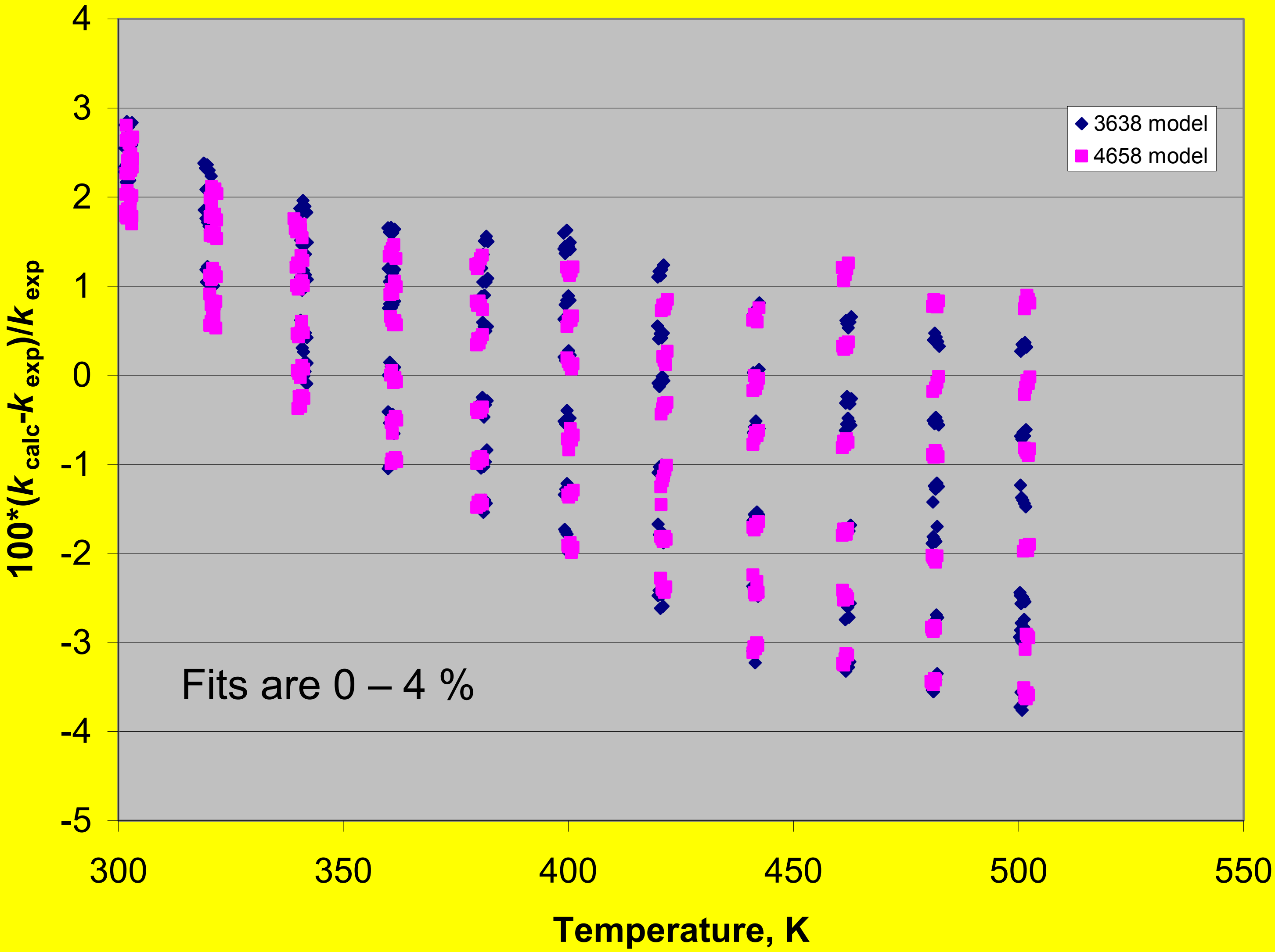
Thermal Conductivity:



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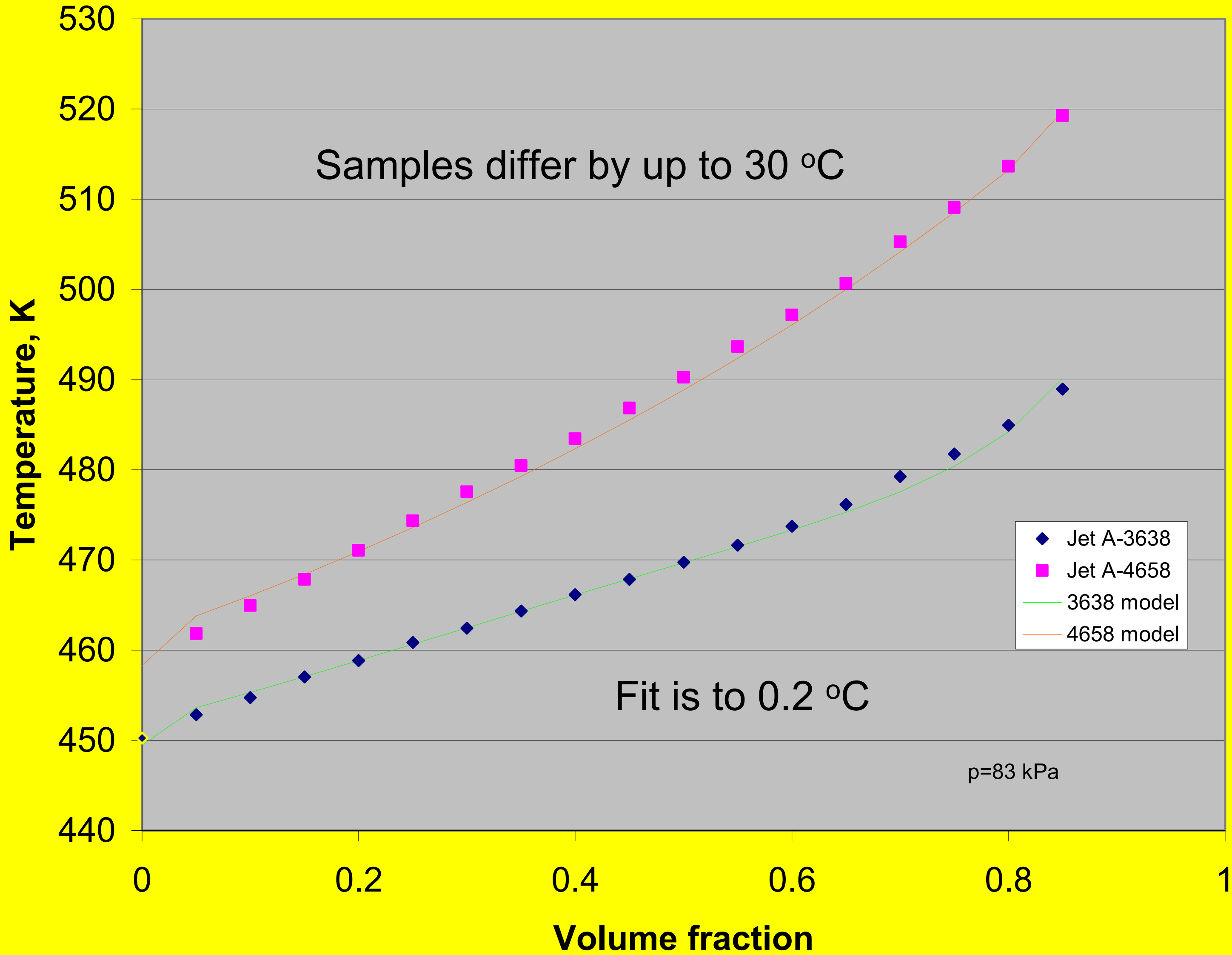
Volatility (ADC):



Conclusions:

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

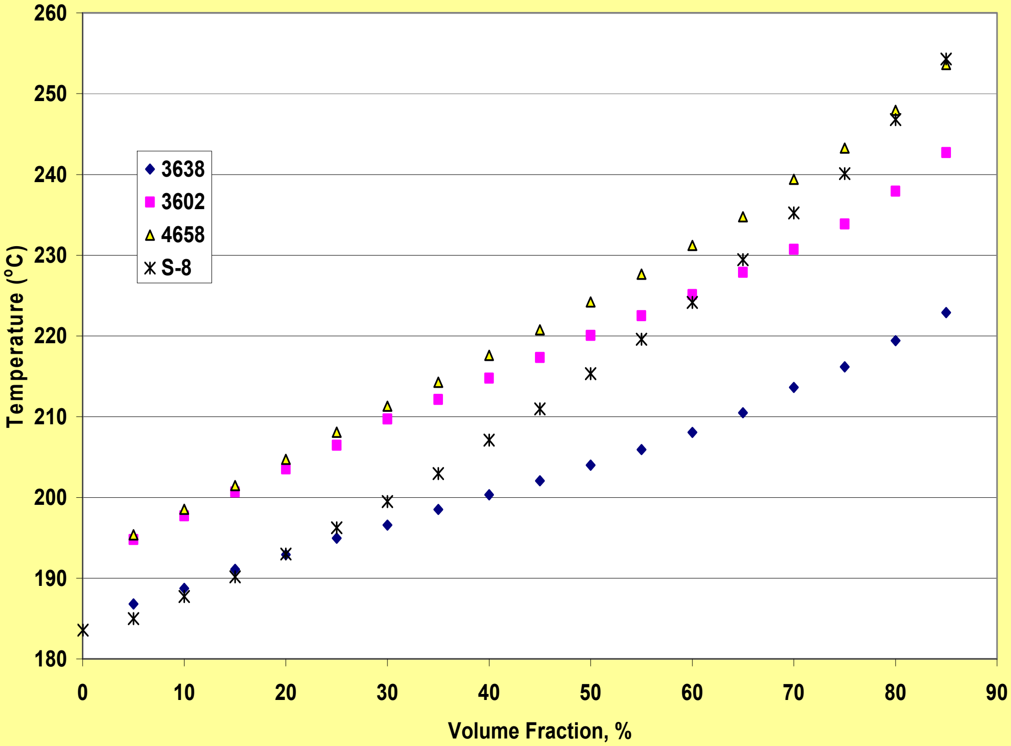
Conclusions:

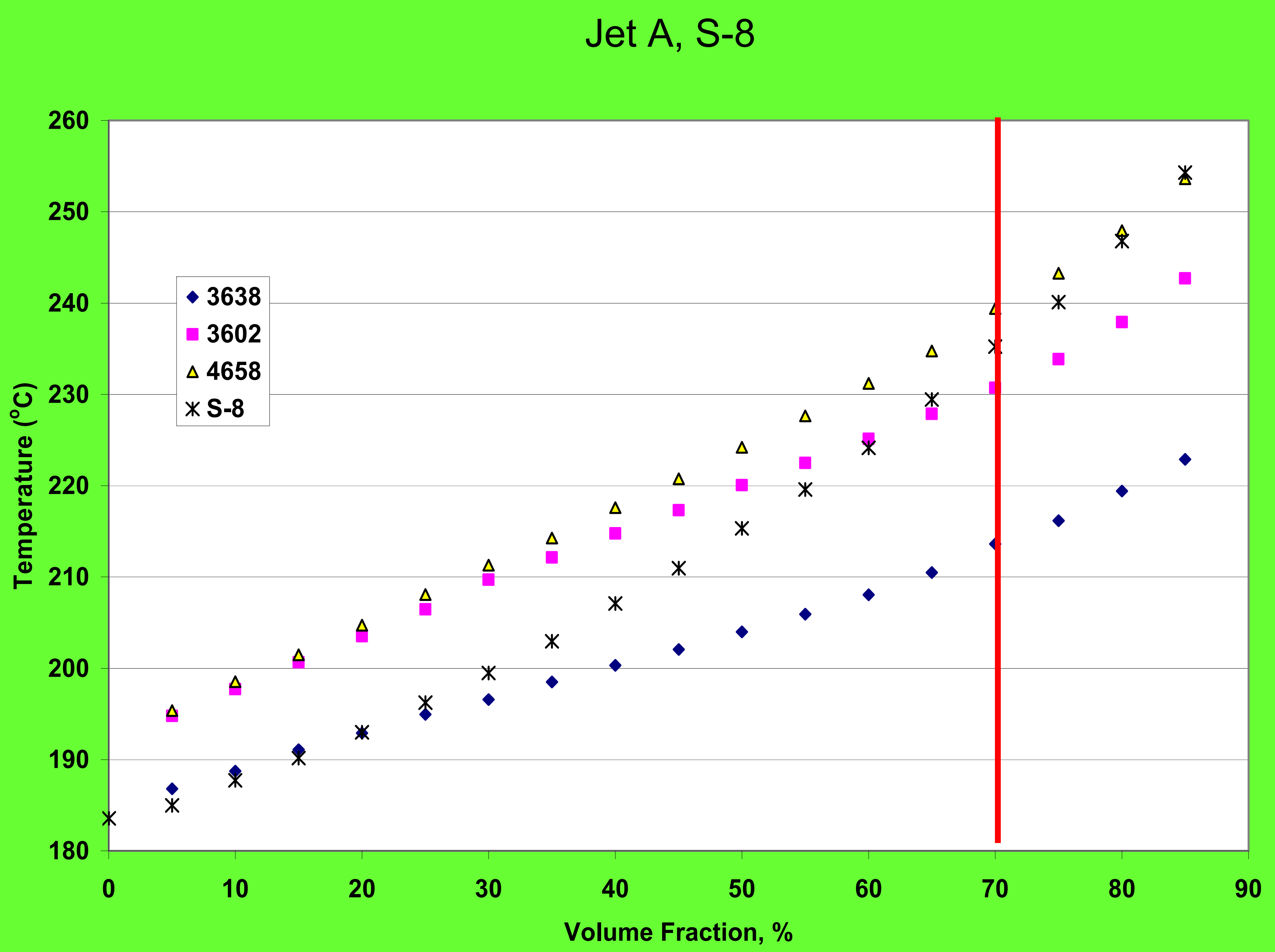
- For most properties, the surrogate models for the “reference JP-8 (Jet-A) represent measurements to experimental uncertainty

- 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:





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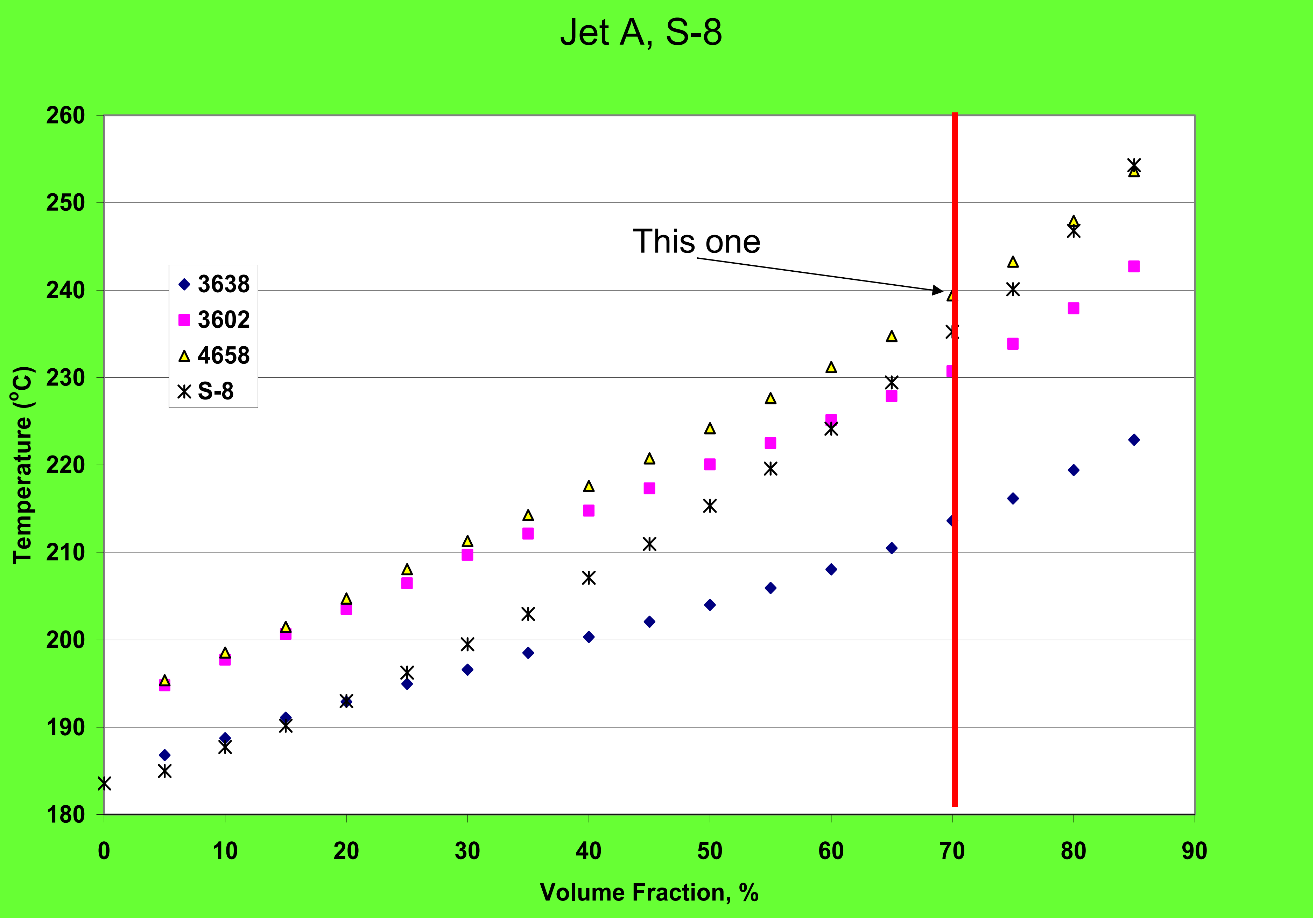
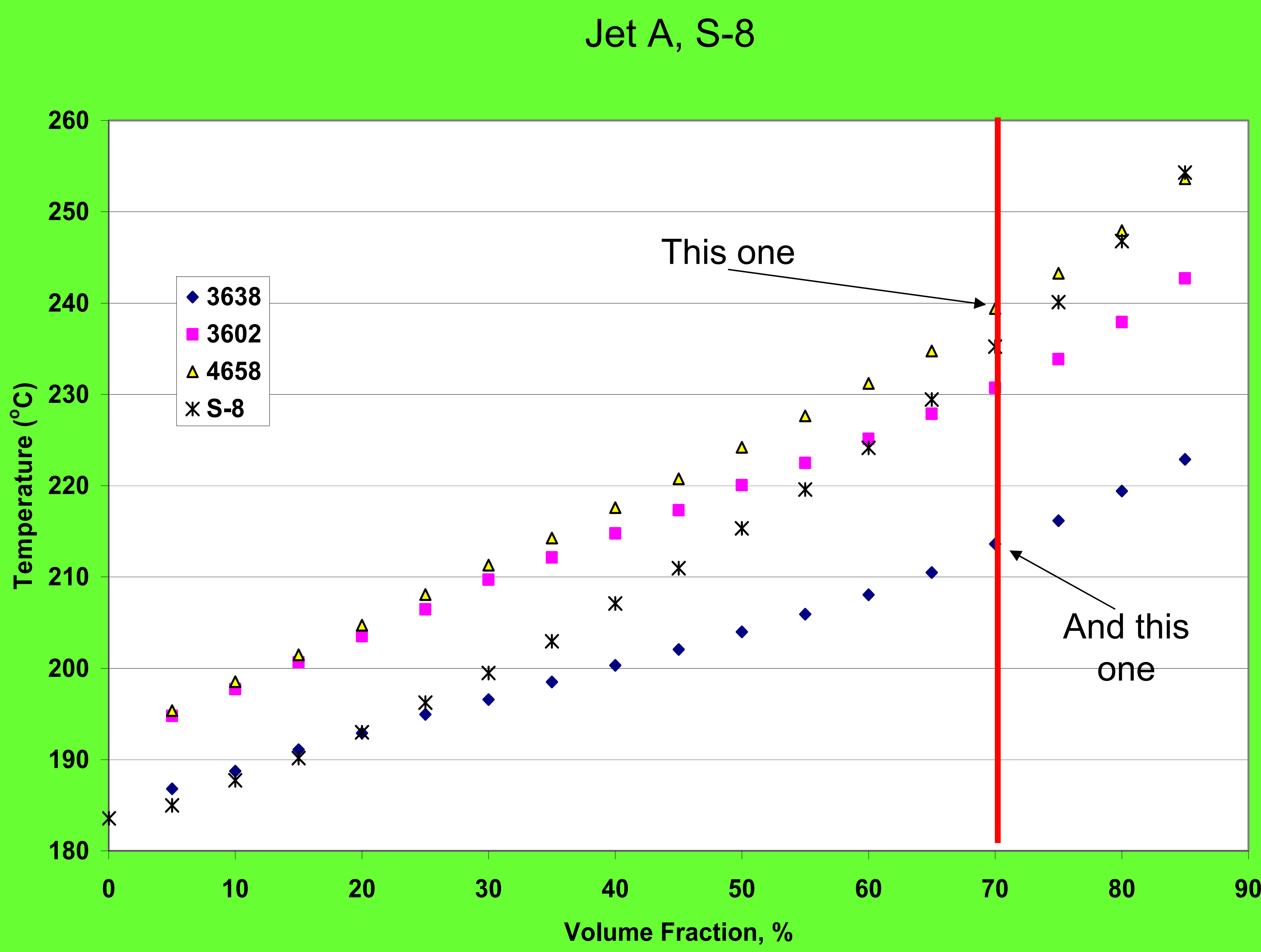
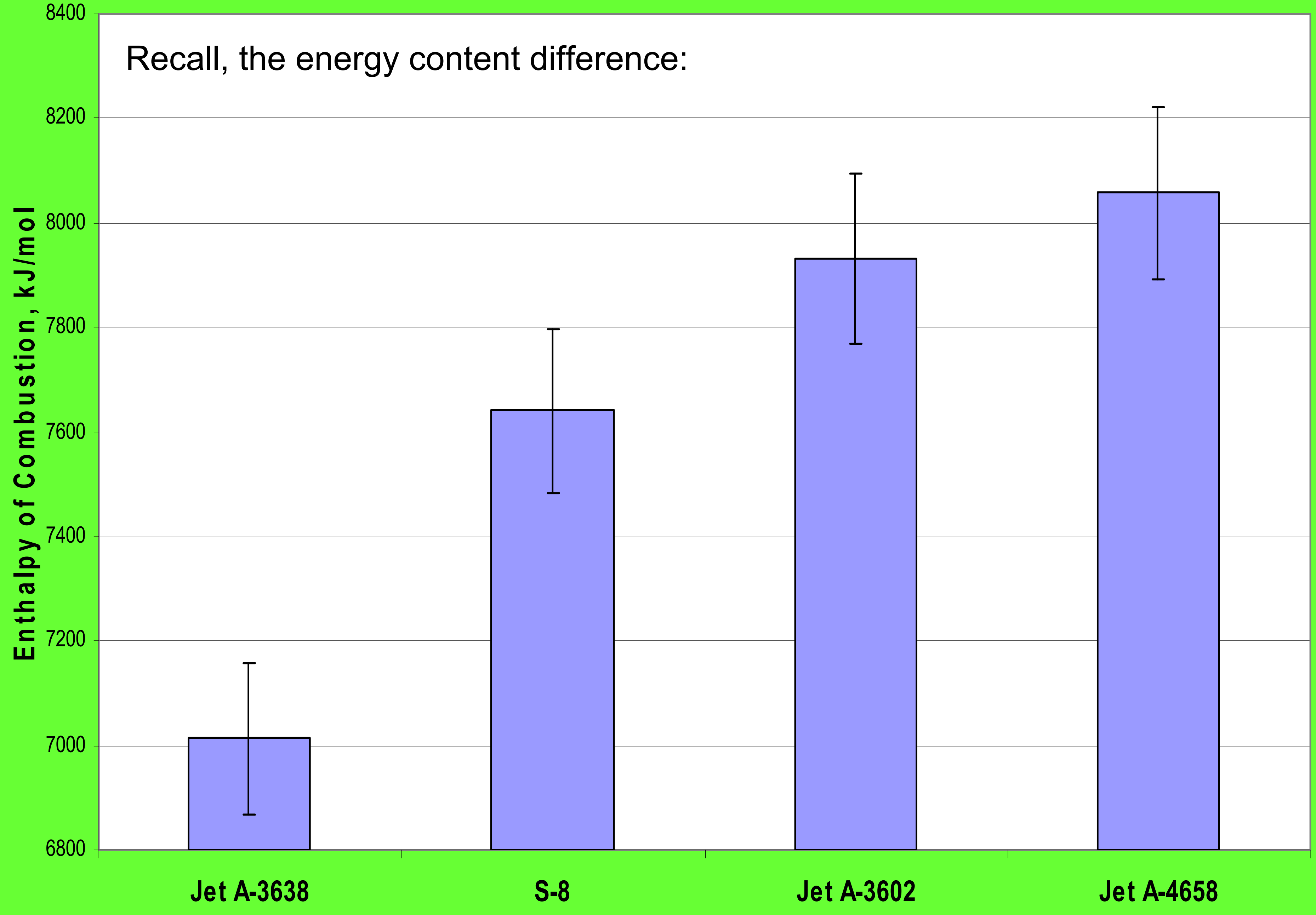

Jet A, S-8
This one
3638
3602
4658
S-8
Temperature (°C)
Volume Fraction, %
260
250
240
230
220
210
200
190
180
0
10
20
30
40
50
60
70
80
90


Jet A, S-8
Temperature (°C)
Volume Fraction, %
3638
3602
4658
S-8
This one
And this one
260
250
240
230
220
210
200
190
180
0
10
20
30
40
50
60
70
80
90



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- 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:

- Bruno, T.J., Method and apparatus for precision on-line sampling of distillate, *Sep. Sci. Tech*., 41, 309-314, 2006.
- Bruno, T.J., Improvements in the measurement of distillation curves. 1. a composition explicit approach, *Ind. Eng. Chem. Res*., 45, 4371-4380, 2006
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- Smith, B.L., Bruno, T.J., Advanced distillation curve measurement with a model predictive temperature controller, *Int. J. Thermophys*., 27, 1419-1434, 2006.
- Bruno, T.J., Smith, B.L., Heat of combustion of fuels as a function of distillate cut: application of an advanced distillation curve method, *Energy and Fuels*, 20, 2109-2116, 2006.
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- Bruno, T.J., The properties of S-8, Final Report for MIPR F4FBEY6237G001, Air Force Research Laboratory, 2006.
- Bruno, T.J., Laesecke, A. Outcalt, S.L., Seelig, H.-D., Smith, B.L., *Properties of a 50/50 Mixture of Jet-A + S-8, NIST-IR-6647, March,* 2007.
- Smith, B.L., Bruno, T.J., Improvements in the measurement of distillation curves: part 3 - application to gasoline and gasoline + methanol mixtures, *Ind. Eng. Chem*. Res., 46, 297-309, 2006.
- Smith, B.L., Bruno, T.J., Improvements in the measurement of distillation curves: part 4- application to the aviation turbine fuel Jet-A, *Ind. Eng. Chem. Res*., 310-320, 2006.

More Documentation:

- Smith, B.L., Bruno, T.J., Composition-explicit distillation curves of aviation fuels JP-8 and the coal-based JP-900, *Energy and Fuels*, 21, 2853-2862, 2007.
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- Huber, M.L., Smith, B.L., Ott, L.S., Bruno, T.J., Surrogate Mixture Model for the Thermophysical Properties of Synthetic Aviation Fuel S-8: Explicit Application of the Advanced Distillation Curve. *Energy & Fuels*, 22**,** 1104 – 1114, 2008.
- Huber, M.L., Lemmon, E.W., Diky, V, Smith, B.L., Bruno, T.J., Chemically authentic surrogate mixture model for the thermophysical properties of a coal-derived-liquid fuel. *Energy and Fuels*, 22, 3249-3257, 2008.
- Widegren, J.A., Bruno, T.J., Thermal decomposition kinetics of the aviation fuel Jet-A. *Ind. Eng. Chem. Res*., 47(13): p. 4342-4348, 2008.
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- Conspicuous by its absence is a paper on the thermodynamic model for JP-8.

- The fuel community should consider this unfinished business.

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