Inevitable Changes in Measurements:
redefining what we mean by “fit-for-purpose”

Thomas J. Bruno

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Boulder, CO

How’s that for a pretentious title?

Experimental Properties of Fluids Group

Welcome

The Experimental Properties of Fluids Group provides the underlying measurement infrastructure for thermodynamic and transport properties of fluids (gaseous and liquid) that is required by industry and government. The Group develops and maintains high accuracy instruments and apparatus for a wide range of pure fluids and fluid mixtures. We cover nonpolar, polar, dipolar aprotic, and aqueous fluids that may consist of one component, or many hundreds of components. Our measurements extend over wide ranges of temperature, pressure and composition. We apply our instrumentation to technically important fluids (fuels, working fluids, etc.) that are critical to industry. All of our work is closely integrated with the activities of the Theory of Fluids Group (which develops thermodynamic and transport property models for fluid properties), and the Thermodynamics Research Center, (which develops the largest thermophysical property databases). Our efforts are leveraged by collaboration with universities, industry consortia, and standards organizations.

In addition to providing the Division's analytical chemistry laboratory, NMR laboratory (Nuclear Magnetic Resonance), and calibration facility, the Group's research activities are in four main areas.

Highlights

NIST paper highlighted in Energy and Fuels Journal

Body of Evidence: New Fast, Reliable Method to Detect Gravesoil

The Joint NIST-AGA Workshop on Odor Masking

Staff

Staff Directory

Alumni

In Memoriam

Staff Speaker Topics

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Programs/Projects

Working/Functional Fluids—The conversion of primary energy (e.g. heat generated by the combustion of a fuel) into useful work most often involves a working fluid operating in a thermodynamic cycle. Examples include a steam …

Energetic Materials—Energetic materials, as distinct from fuels, include explosives, propellants and ignitable liquids. One typically associates the study of energetic materials with forensics, in the …

Fuels—Energy is one of the most critical problems facing the United States, with technical, economic and public policy aspects. Decision makers depend on reliable and objective characterization of fuels …

Standard Reference Fluid Measurements—Property measurements of the very highest accuracies are important for developing the thermodynamic and transport property models for working fluids and reference fluids. More than simply providing …

Fit-for-Purpose:

- A capstone of QA principles
  - product should be suitable for the intended purpose

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    - **fulfilling** a customer’s requirements, needs or desires
    - whether or not a unit **meets quality**
    - resources should not be **squandered** to produce higher quality than is necessary
    - **conform** to generally accepted standards (accreditation or quality assurance body)
    - "in spec" or "out of spec"

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      - Test methods and procedures
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      - Cost, simplicity driven
- Development driven by what can be measured

An Alternative:

- Fundamental Properties, rather than “fit-for-purpose” properties

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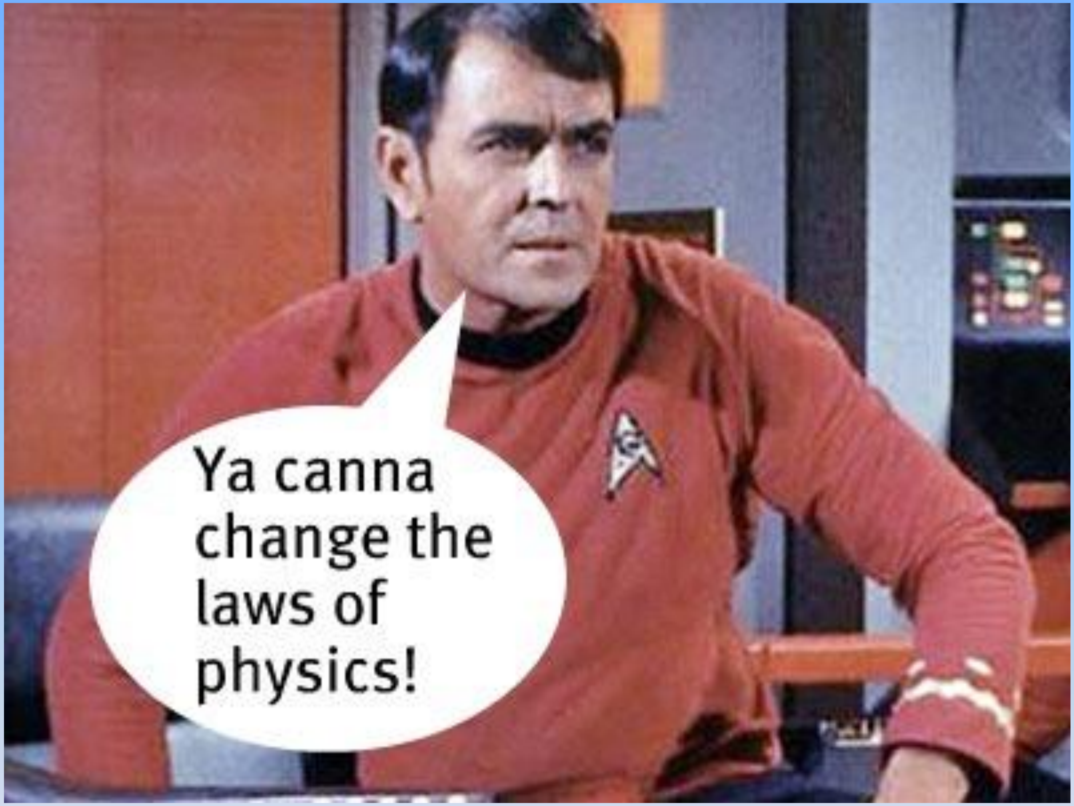
  - Fundamental properties are linked to fundamental theory
    - Math ⟷ Measurement

An Alternative:

- Fundamental Properties, rather than “fit-for-purpose” properties
  - Fundamental properties are linked to fundamental theory
    - Math ⟷ Measurement
  - Fundamental properties derive from atoms and molecules
    - Explicit recognition that composition determines property


Ya canna change the laws of physics!

Fuel Test Methods:

- Volatility
- Vapor Pressure
- Cetane index
- Antiknock index
- Gravity
- Acidity
- Color
- etc., etc….

At the top of the list for good reasons!

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)

Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure[1]

This standard is issued under the fixed designation D 86; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

This specification has been approved for use by agencies of the Department of Defense.

1. Scope[2]

1.1 This test method covers the atmospheric distillation of petroleum products using a laboratory batch distillation unit to determine quantitatively the boiling range characteristics of such products as natural gasolines, light and middle distillates, automotive spark-ignition engine fuels, aviation gasolines, aviation turbine fuels, 1-D and 2-D regular and low sulfur diesel fuels, special petroleum spirits, naphthas, white spirits, kerosines, and Grades 1 and 2 burner fuels.

1.2 The test method is designed for the analysis of distillate fuels; it is not applicable to products containing appreciable quantities of residual material.

1.3 This test method covers both manual and automated instruments. In cases of dispute, the manual apparatus and procedure shall be the referee test method.

1.4 Unless otherwise noted, the values stated in SI units are to be regarded as the standard. The values given in parentheses are provided for information only.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 All standards are subject to revision, and parties to agreement on this test method are to apply the most recent edition of the standards indicated below, unless otherwise specified, such as in contractual agreements or regulatory rules, where earlier versions of the method(s) identified may be required.

2.2 *ASTM Standards:*

D 97 Test Method for Pour Point of Petroleum[3]
D 323 Test Method for Vapor Pressure of Petroleum Products (Reid Method)[3]
D 850 Test Method for Distillation of Industrial Aromatic Hydrocarbons and Related Materials[4]
D 1078 Test Method for Distillation Range of Volatile Organic Liquids[4]
D 2892 Test Method for Distillation of Crude Petroleum (15-Theoretical Plate Column)[5]
D 4057 Practice for Manual Sampling of Petroleum and Petroleum Products[5]
D 4177 Practice for Automatic Sampling of Petroleum and Petroleum Products[5]
D 4953 Test Method for Vapor Pressure of Gasoline and Gasoline Oxygenate Blends (Dry Method)[6]
D 5190 Test Method for Vapor Pressure of Petroleum Products (Automatic Method)[6]
D 5191 Test Method for Vapor Pressure of Petroleum Products (Mini Method)[6]
D 5482 Test Method for Vapor Pressure of Petroleum Products (Mini Method-Atmospheric)[6]
D 5949 Test Method for Pour Point of Petroleum Products (Automatic Pressure Pulsing Method)[6]
D 5950 Test Method for Pour Point of Petroleum Products (Automatic Tilt Method)[6]
D 5985 Test Method for Pour Point of Petroleum Products (Rotational Method)[6]
E 1 Specification for ASTM Thermometers[7]
E 77 Test Method for Inspection and Verification of Thermometers[7]
E 1272 Specification for Laboratory Glass Graduated Cylinders[8]
E 1405 Specification for Laboratory Glass Distillation Flasks[8]

2.3 *IP Standards:*[9]

IP 69 Determination of Vapour Pressure—Reid Method
IP 123 Petroleum Products—Determination of Distillation Characteristics
IP 394 Determination of Air Saturated Vapour Pressure
IP Standard Methods for Analysis and Testing of Petroleum and Related Products 1996—Appendix A

3. Terminology

3.1 *Definitions:*

3.1.1 *charge volume, n*—the volume of the specimen, 100 mL, charged to the distillation flask at the temperature specified in Table 3.

3.1.2 *decomposition, n—of a hydrocarbon*, the pyrolysis or cracking of a molecule yielding smaller molecules with lower boiling points than the original molecule.

3.1.2.1 *decomposition point, n*—the corrected thermom-

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[1] This test method is under the jurisdiction of ASTM Committee D-2 on Petroleum Products and Lubricants and is the direct responsibility of Subcommittee D02.08 on Volatility.

In the IP, the equivalent test method is published under the designation IP 123. It is under the jurisdiction of the Standardization Committee.

Current edition approved Nov. 10, 1997. Published February 1998.

[2] This test method is a complete rewrite of D 86 – 96.

[3] *Annual Book of ASTM Standards*, Vol 05.01.

[4] *Annual Book of ASTM Standards*, Vol 06.04.

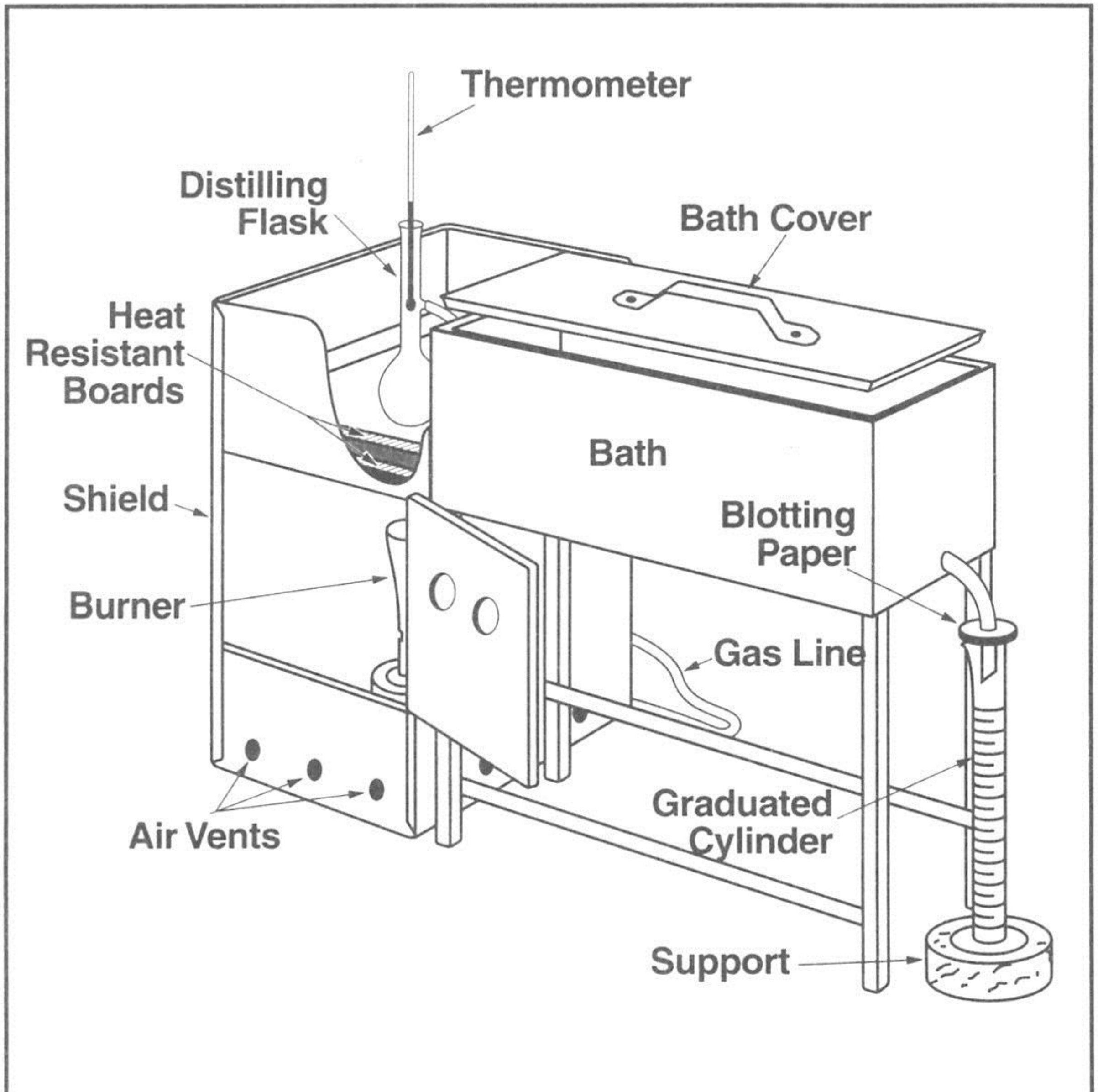
[5] *Annual Book of ASTM Standards*, Vol 05.02.

[6] *Annual Book of ASTM Standards*, Vol 05.03.

[7] *Annual Book of ASTM Standards*, Vol 14.03.

[8] *Annual Book of ASTM Standards*, Vol 14.02.

[9] Available from the Institute of Petroleum, 61 New Cavendish St., London, W1M 8AR, UK.

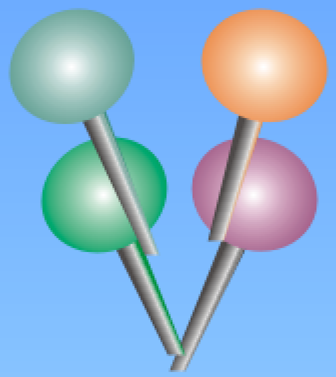

Thermometer
Distilling Flask
Bath Cover
Heat Resistant Boards
Bath
Shield
Blotting Paper
Burner
Gas Line
Graduated Cylinder
Air Vents
Support

Anything Wrong with it?

- The D-86 distillation curve has no basis in theory, and cannot be modeled.
  - temperatures are not thermodynamic state points
  - value comes from standardization

- Numerous sources of uncertainty in T and V

- Initial boiling temperature is invalid
  - first drop at the receiver
  - boiling starts long before this
  - error (systematic) is 7-15 °C



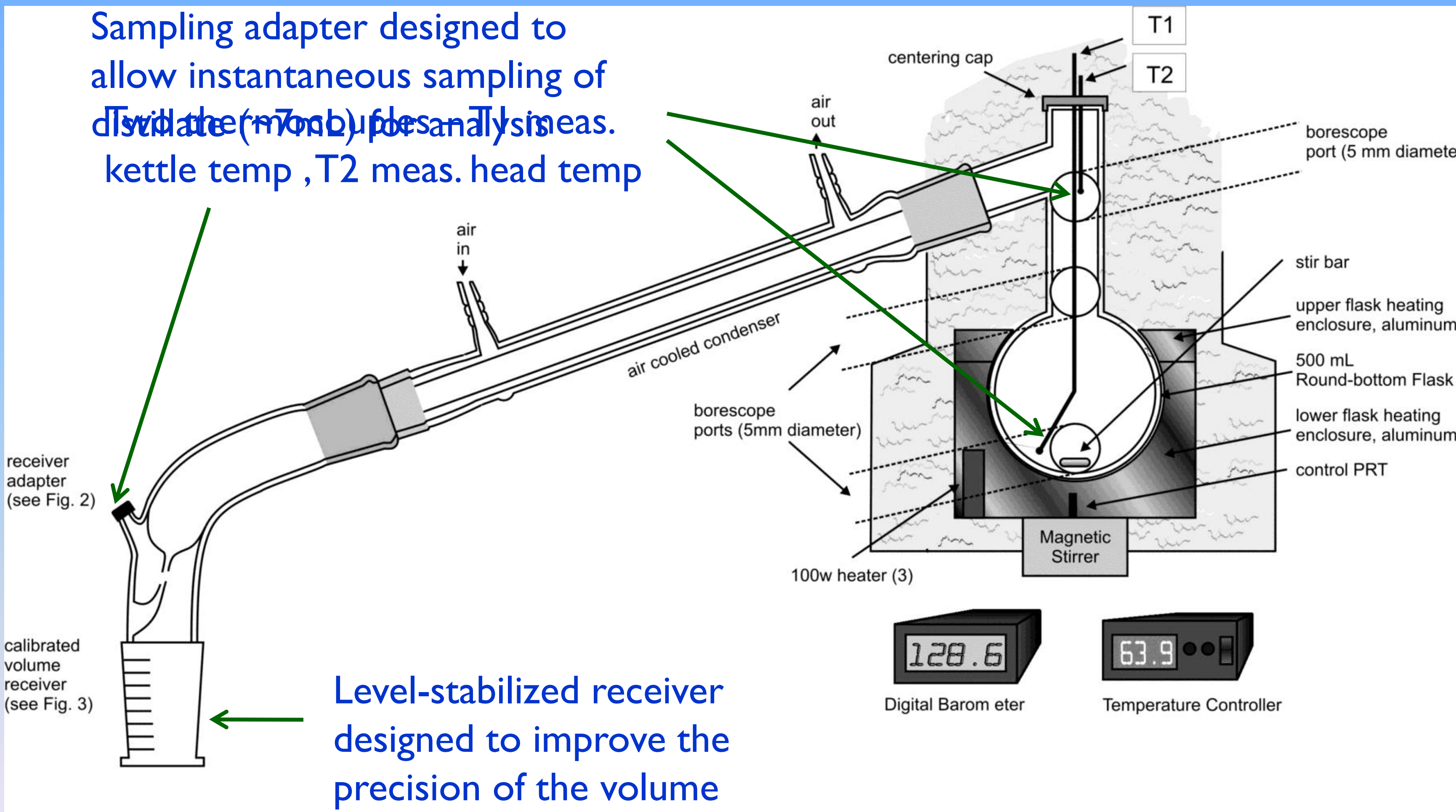
Standardized Voodoo

- Dr. Willie E. May, NIST

ADC Analytical Protocol for 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
- Explicit identification of **azeotropes**
- **energy content** of each fraction
- **corrosivity** of each fraction
- **greenhouse** gas output of each fraction
- thermal and oxidative **stability** of the fluids

Advanced Distillation Curve (ADC) Apparatus

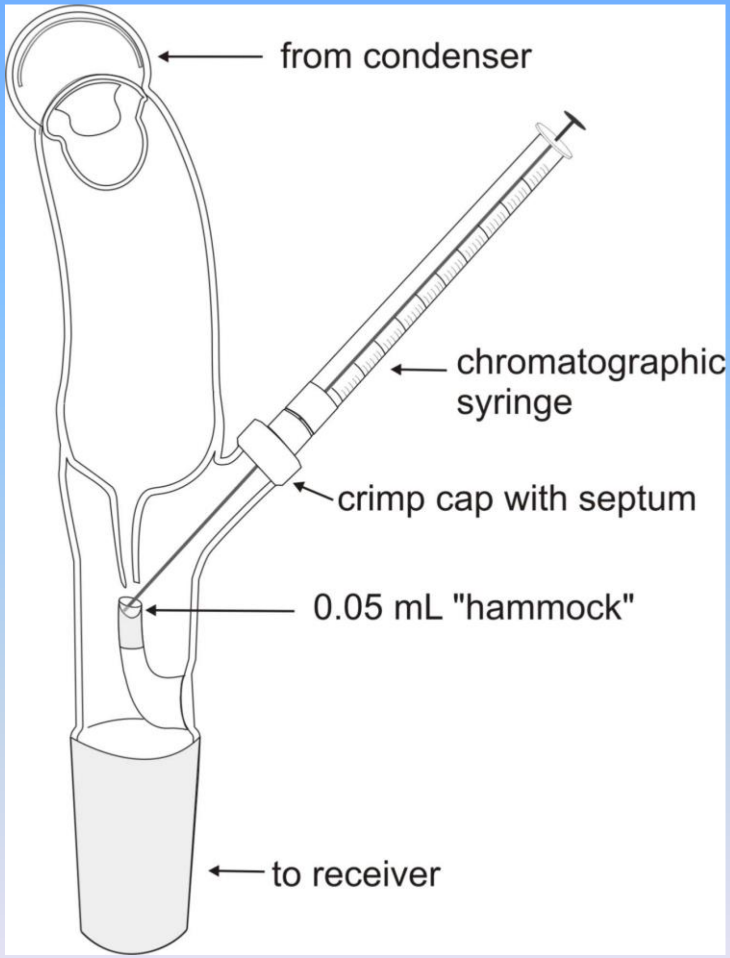


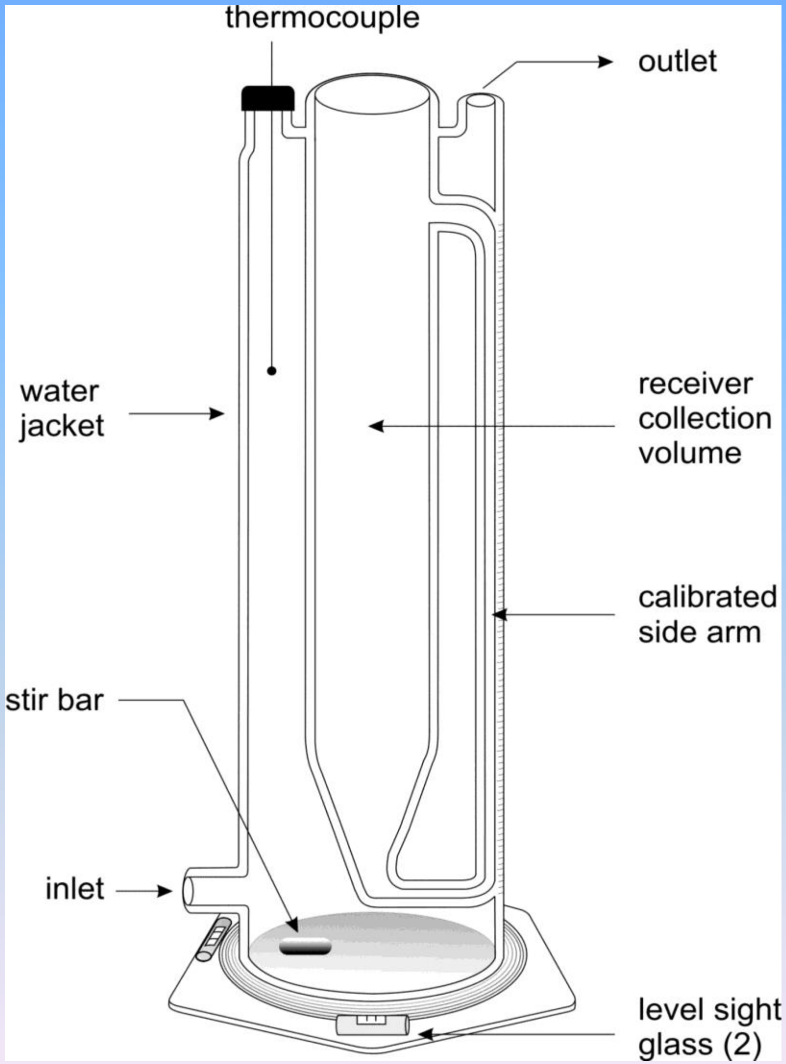
Sampling adapter designed to allow instantaneous sampling of distillate (~7mL) for analysis

Two thermocouples – T1 meas. kettle temp , T2 meas. head temp

Level-stabilized receiver designed to improve the precision of the volume measurement

Sampling Adapter & Level Stabilized Receiver



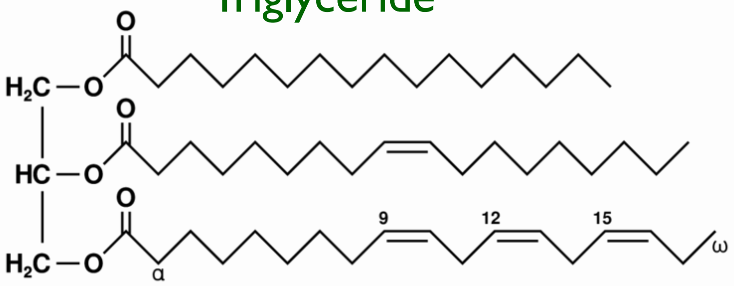


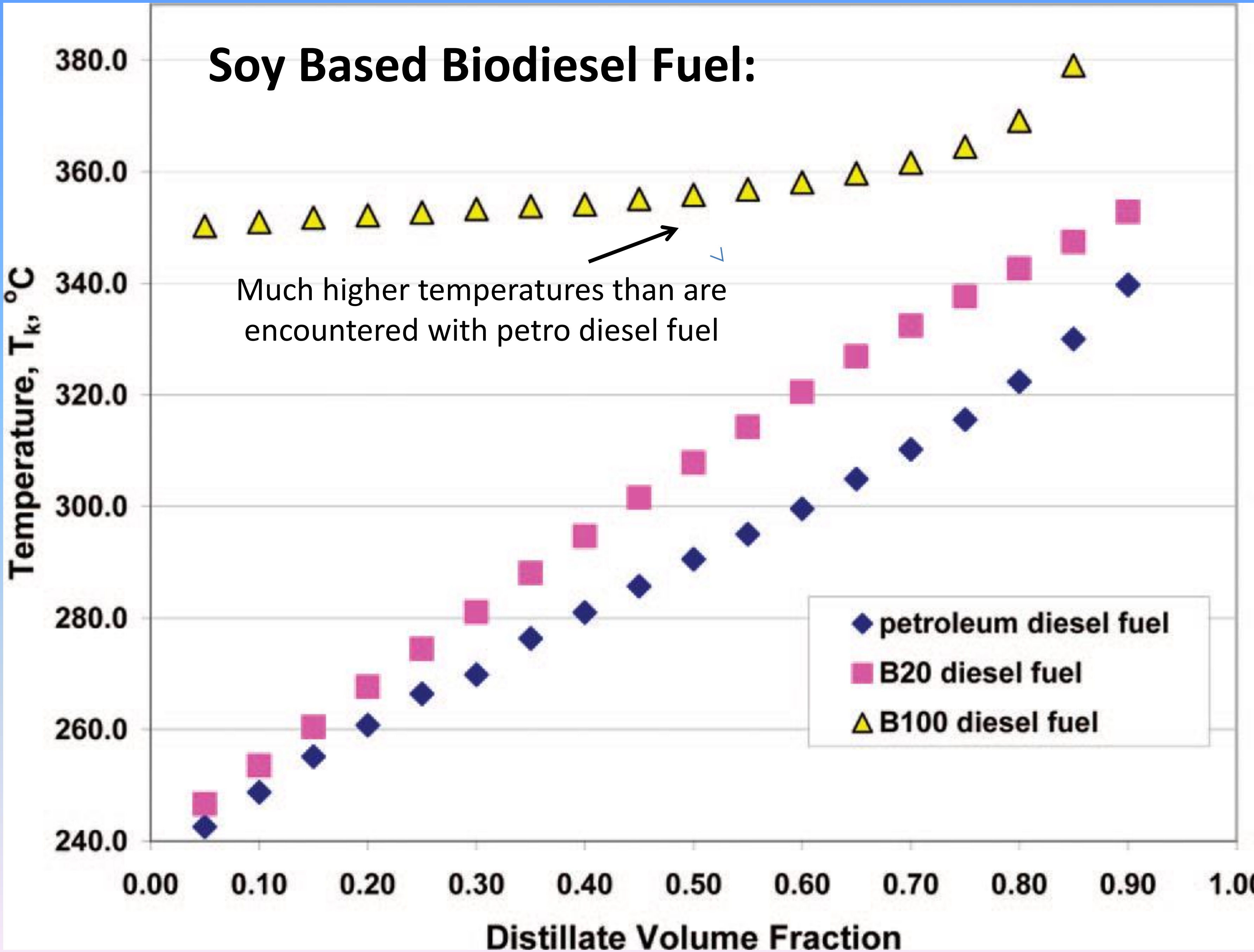
Commercialized by Sigma Aldrich

Choosing a Biodiesel Fuel Feedstock

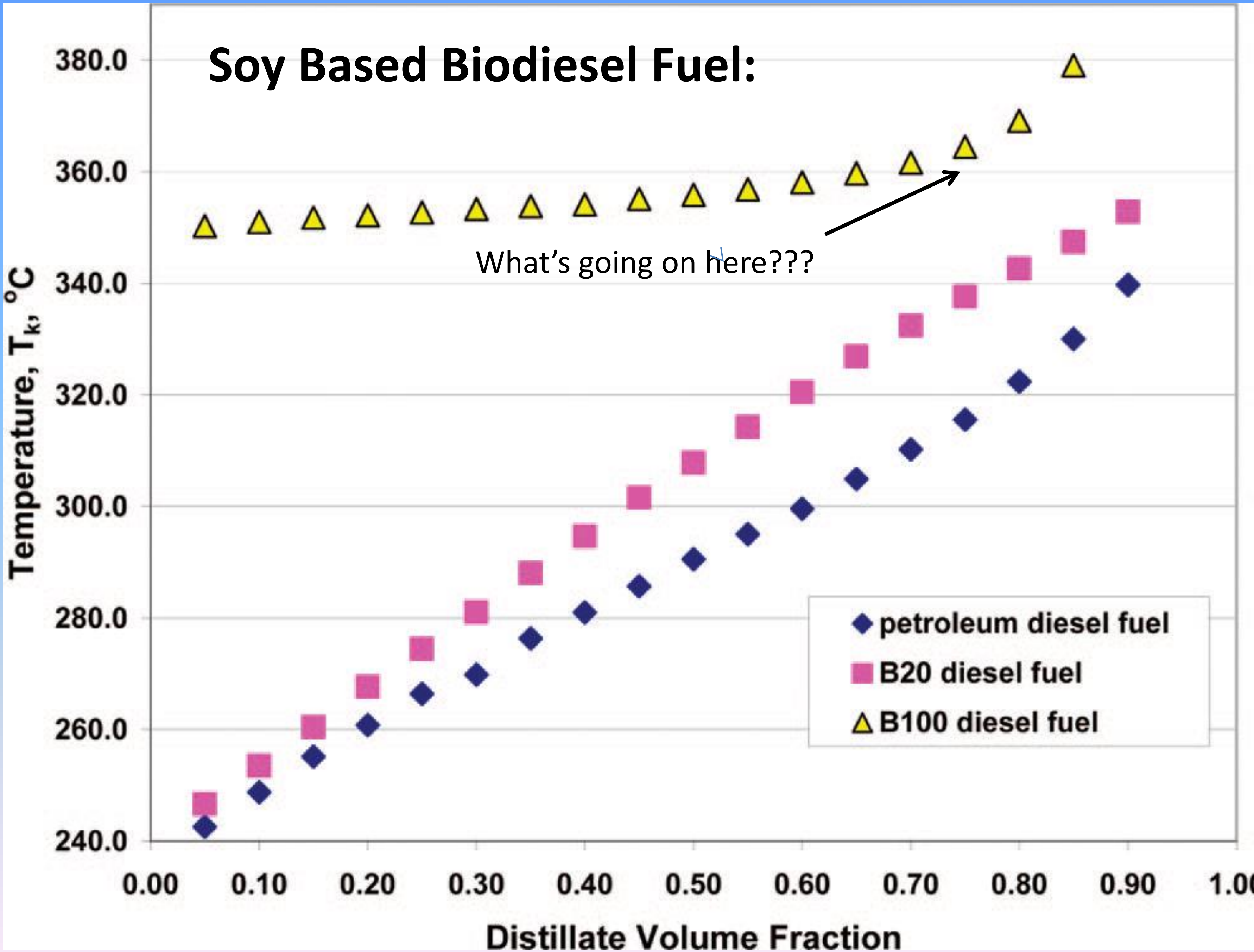
- Grown locally
  - geography
  - climate
  - availability
- Feedstock oil determines
  - fatty acid content
  - FAME profile (composition and degree of unsaturation)
  - resulting properties of the biodiesel fuel
    - cold flow properties
    - oxidative stability
    - energy content

Triglyceride





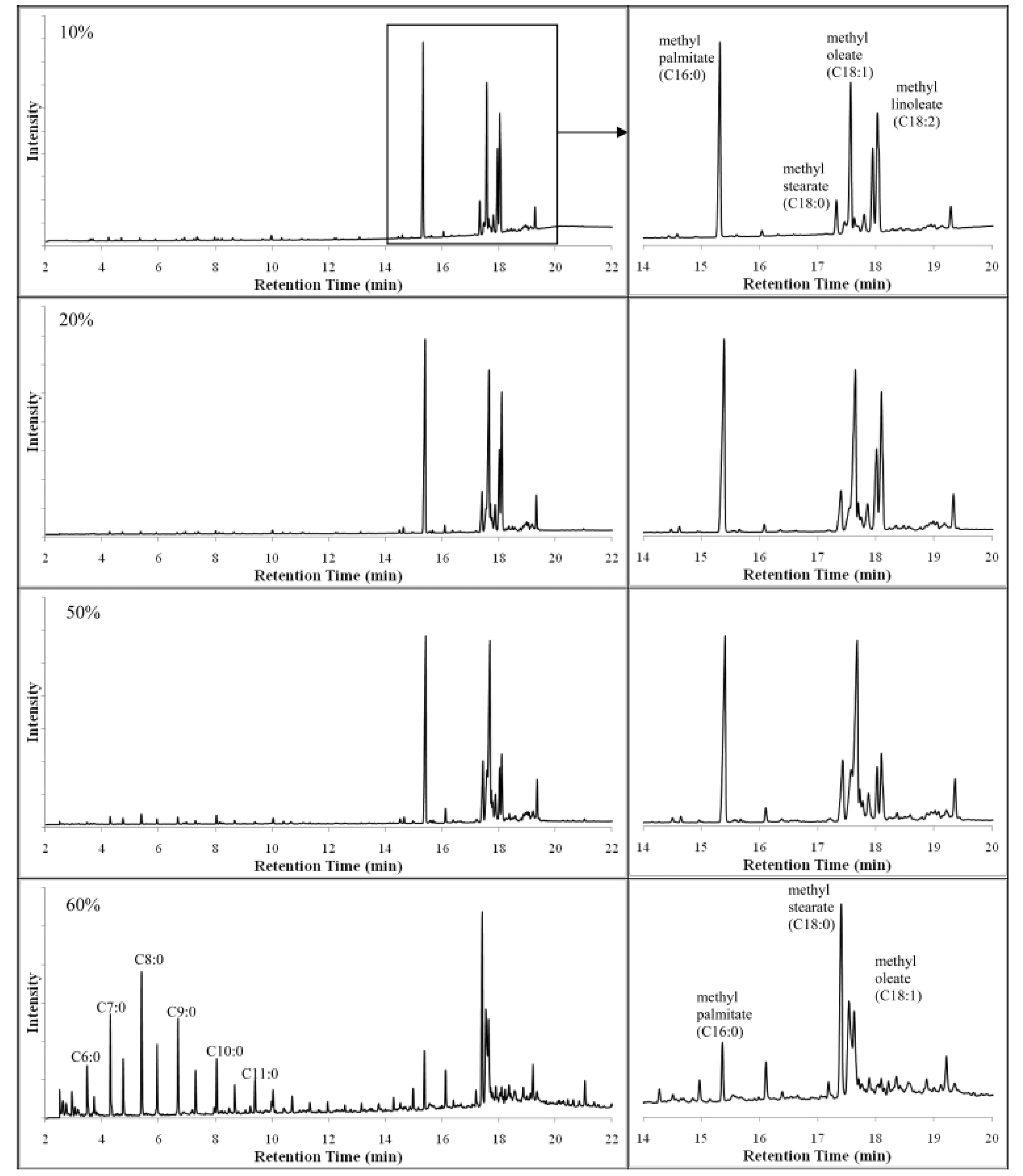
Soy Based Biodiesel Fuel:
Much higher temperatures than are
encountered with petro diesel fuel
Temperature, T_k, °C
380.0
360.0
340.0
320.0
300.0
280.0
260.0
240.0
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
Distillate Volume Fraction
petroleum diesel fuel
B20 diesel fuel
B100 diesel fuel



Soy Based Biodiesel Fuel:
What's going on here???
Temperature, T_k, °C
380.0
360.0
340.0
320.0
300.0
280.0
260.0
240.0
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
Distillate Volume Fraction
petroleum diesel fuel
B20 diesel fuel
B100 diesel fuel

Use the composition explicit data channel to find out

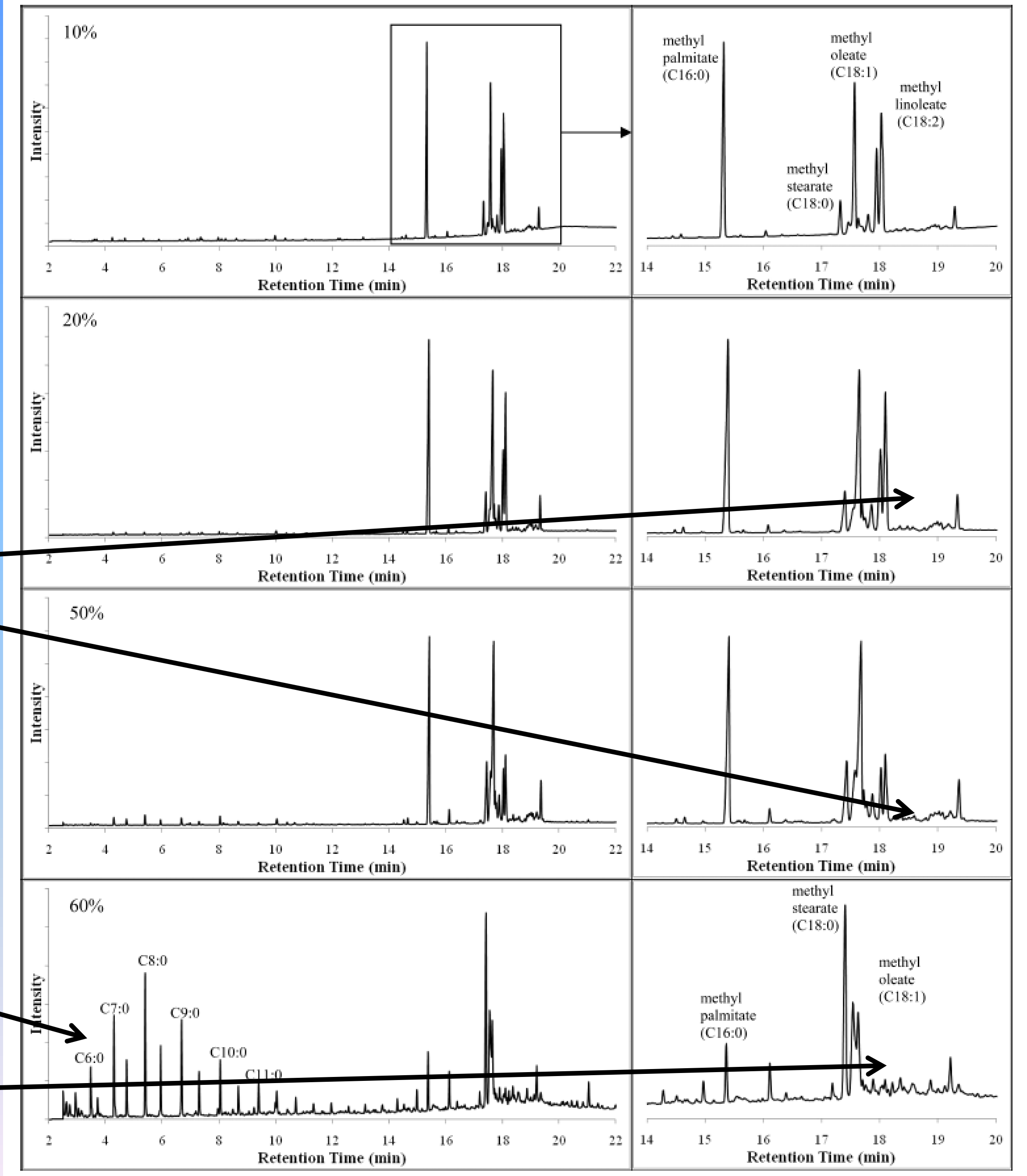
Diels Alder products forming



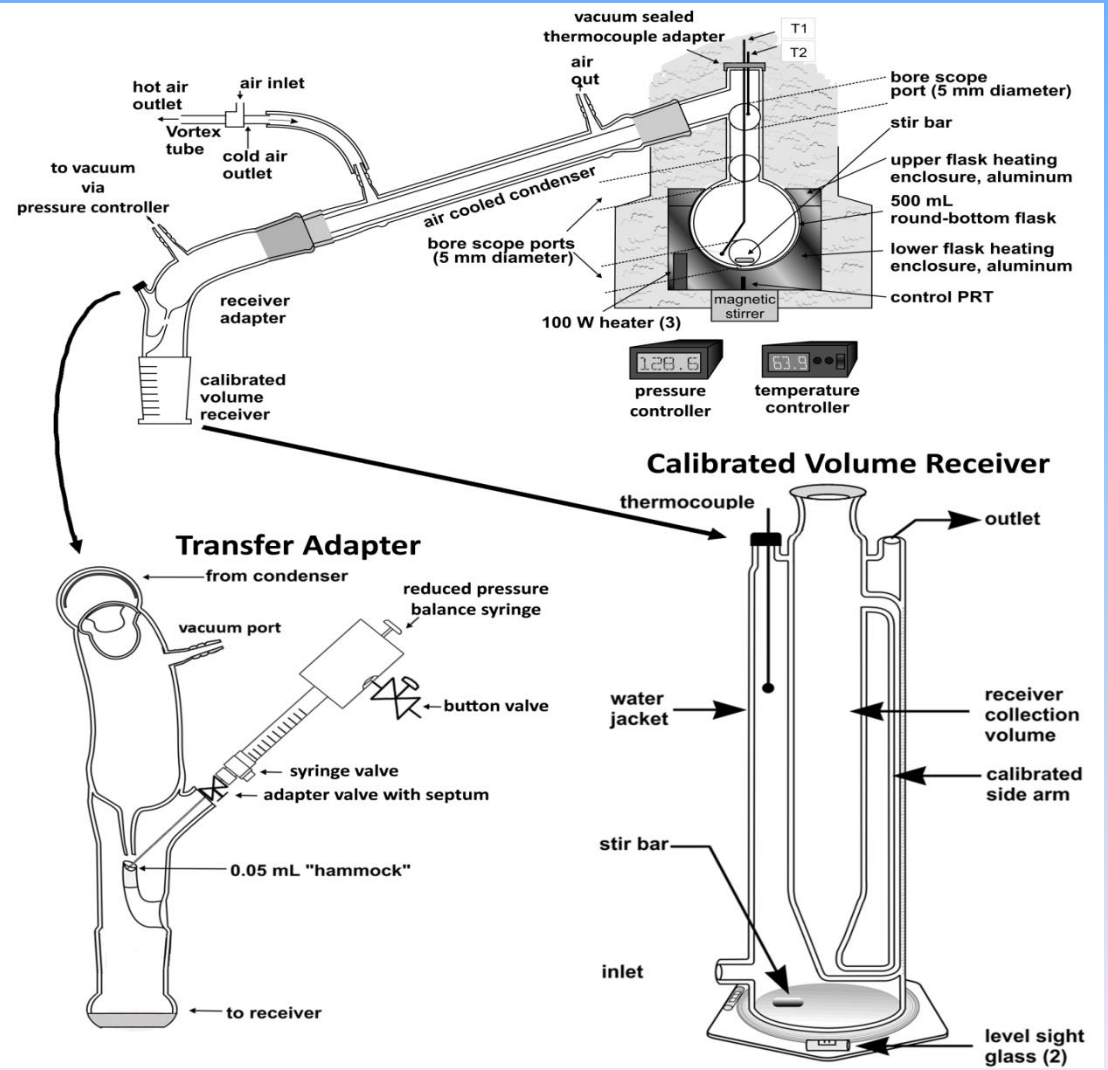
Use the composition explicit data channel to find out

Diels Alder products forming

Cracking products and lots of Diels Alder products



Lower the Pressure, Lower the Temperature

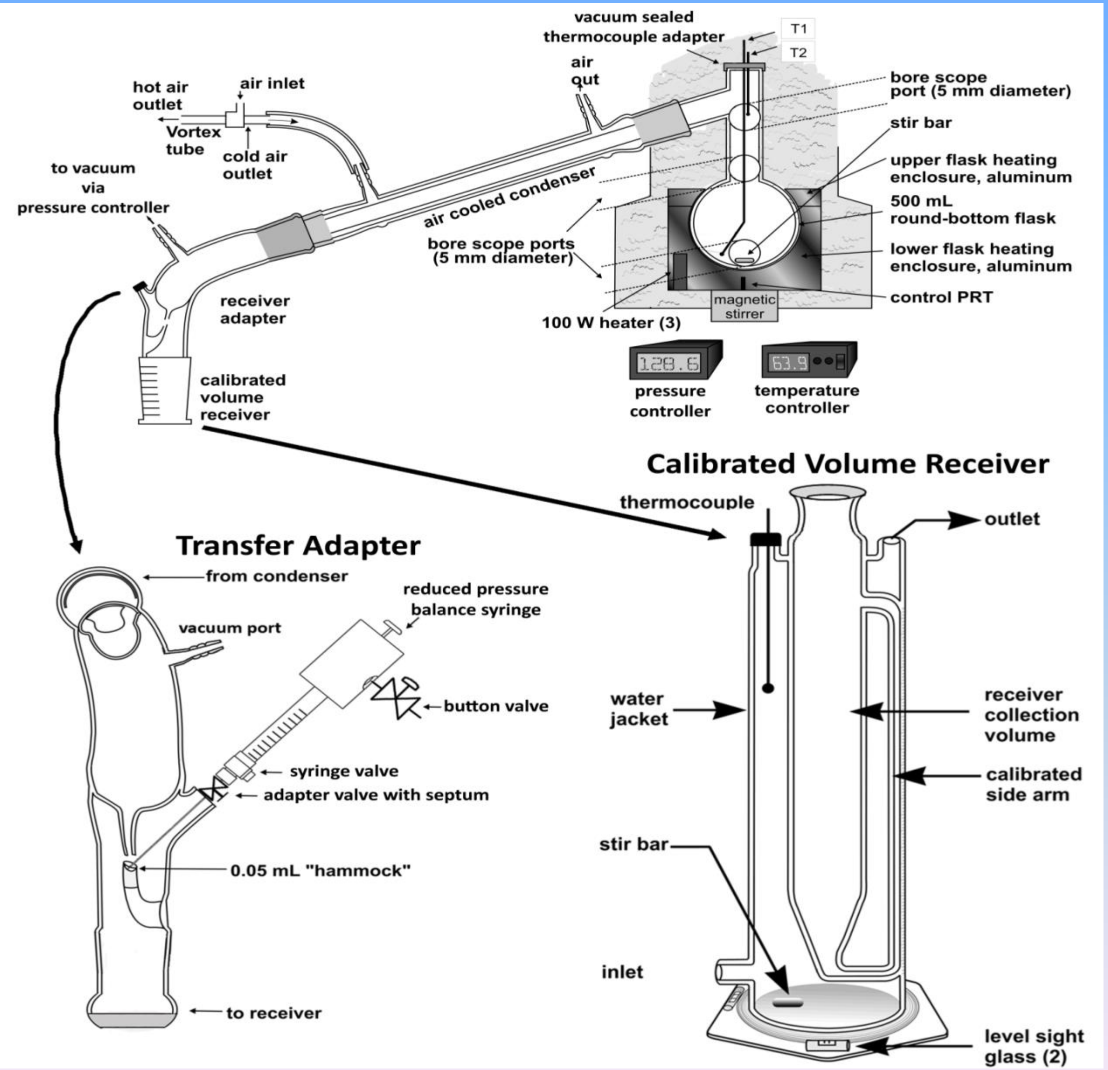


Lower the Pressure, Lower the Temperature

Apparatus is vacuum tight,

with a PID vacuum controller,

CO_2 controlled.



Lower the Pressure, Lower the Temperature

Apparatus is vacuum tight,

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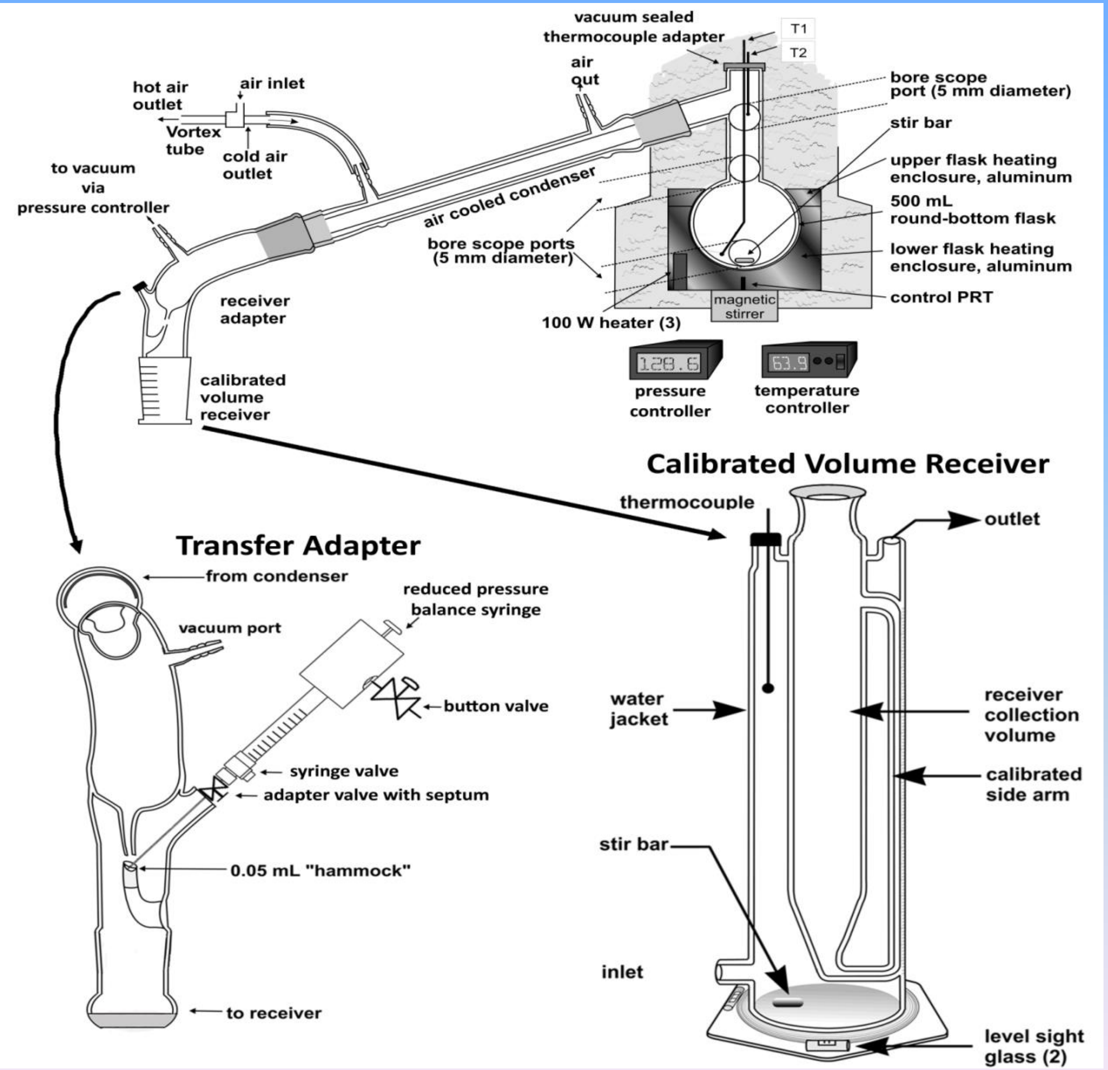
A low pressure, pressure balanced syringe for sampling



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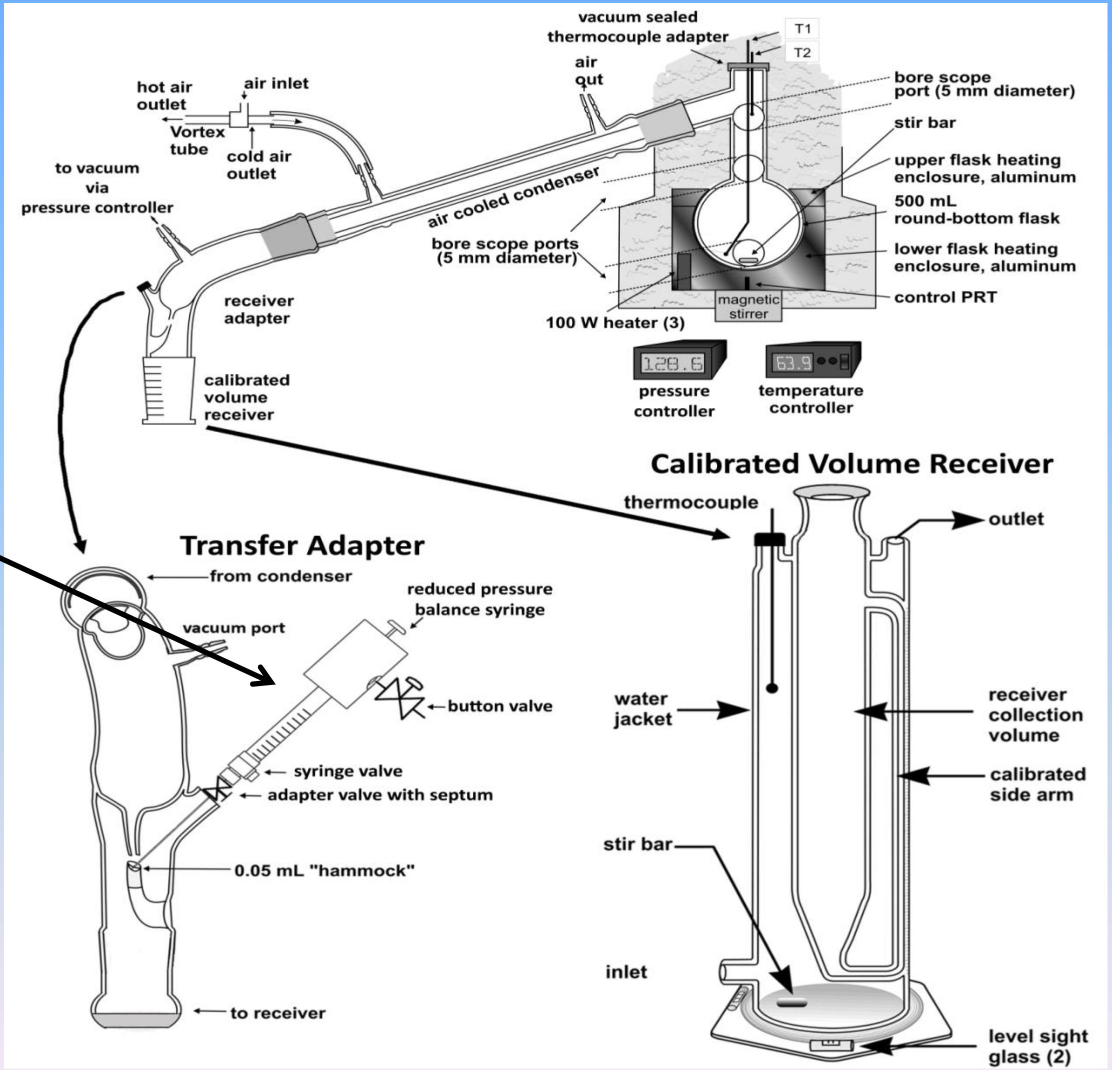
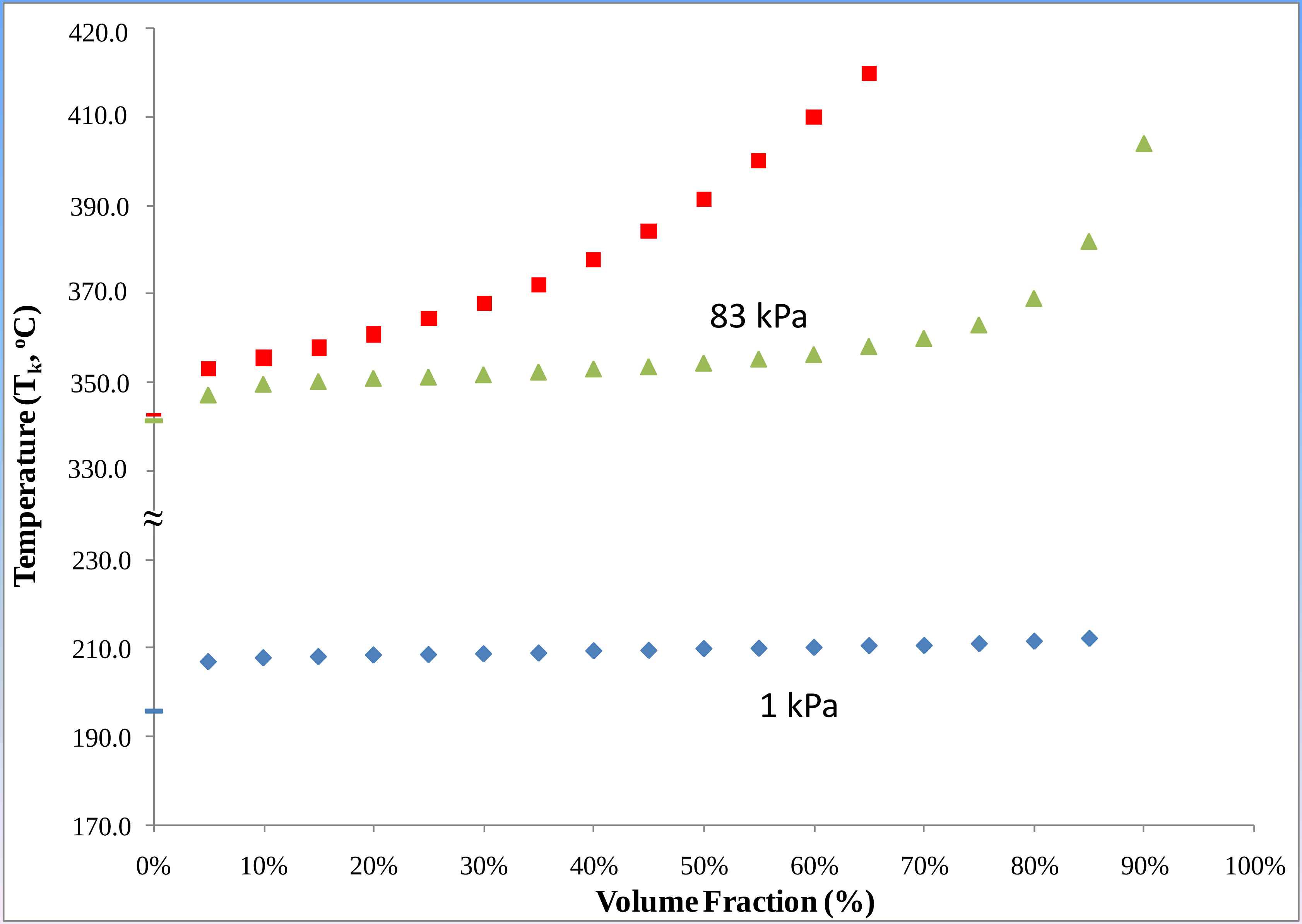
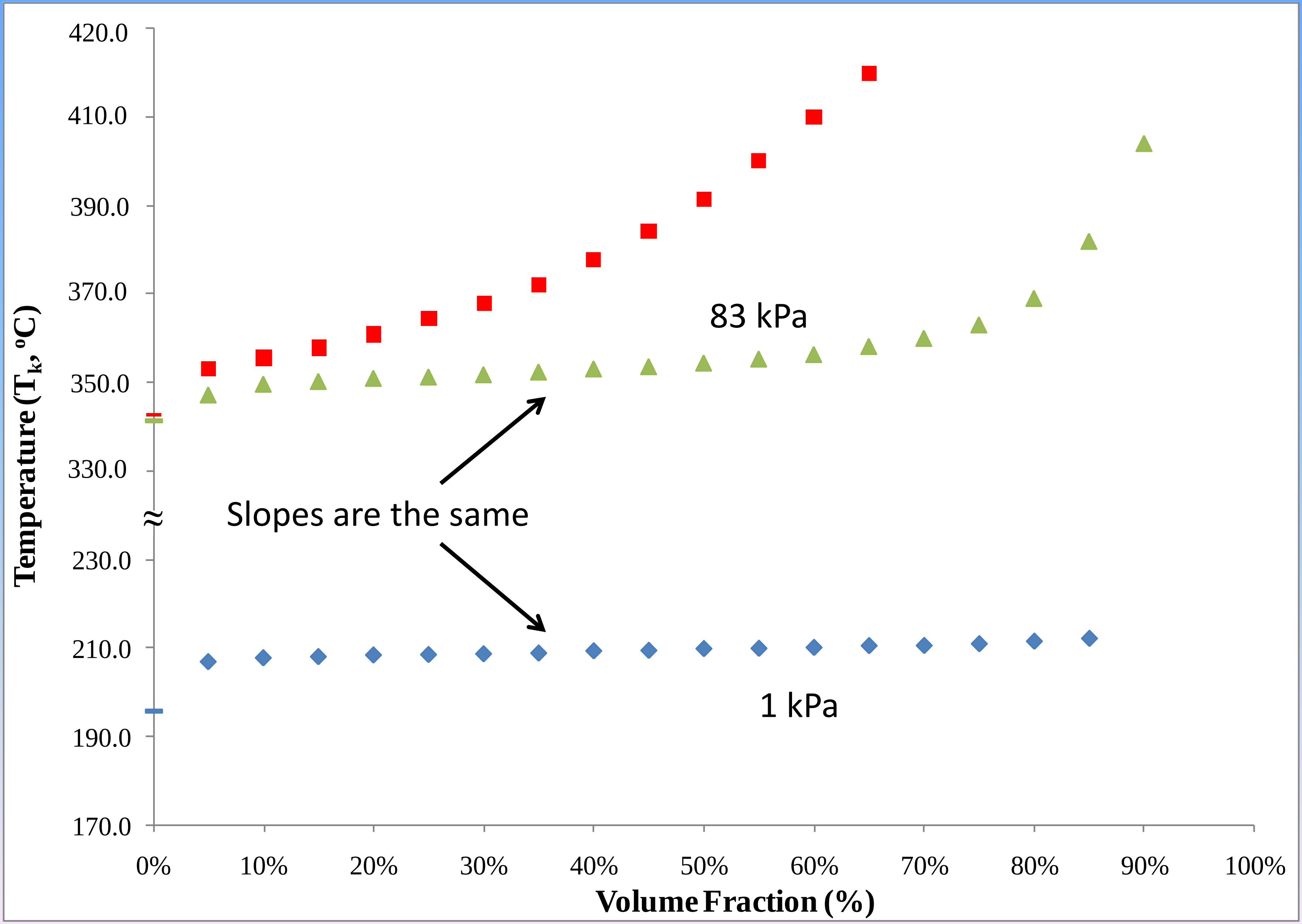
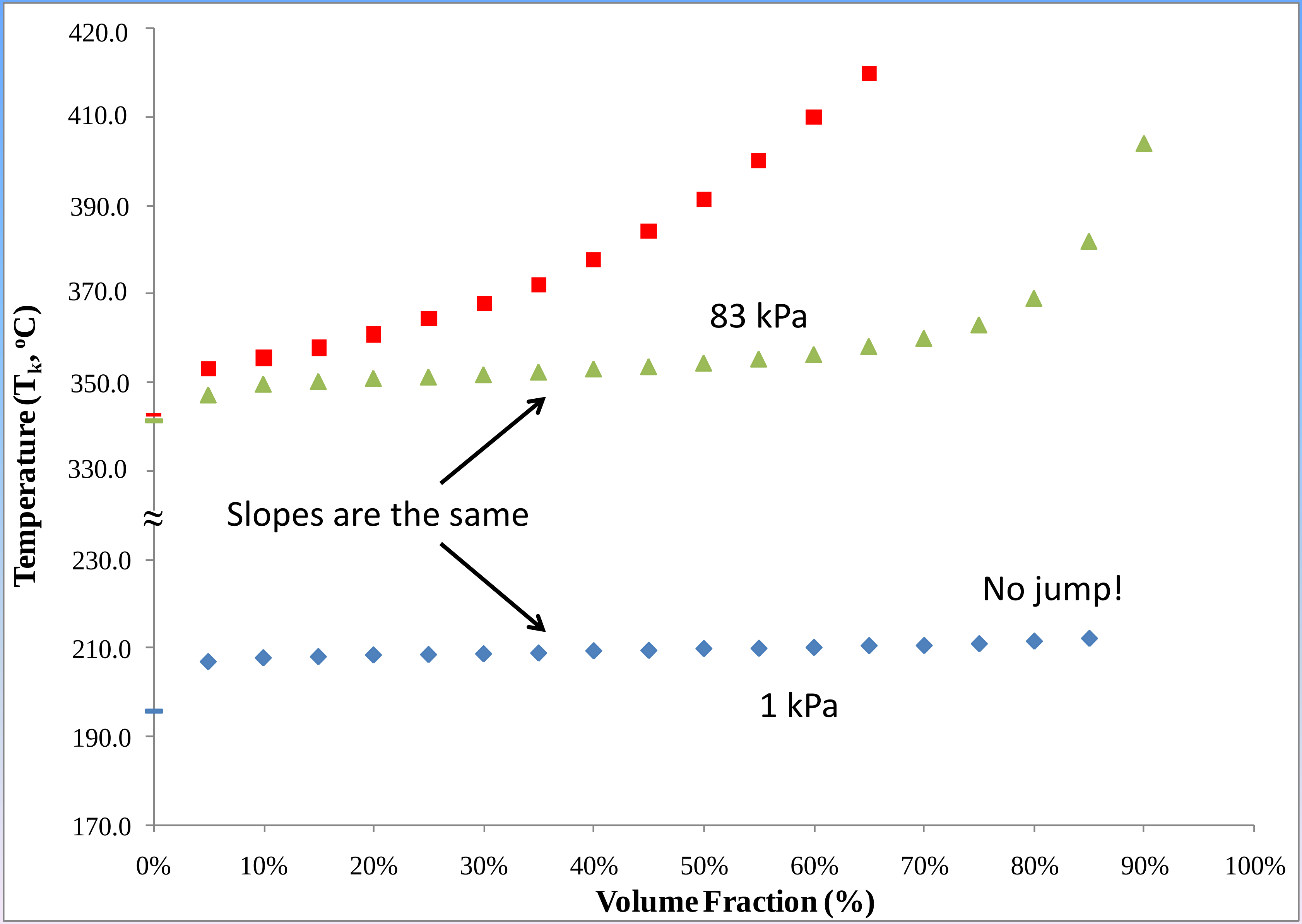


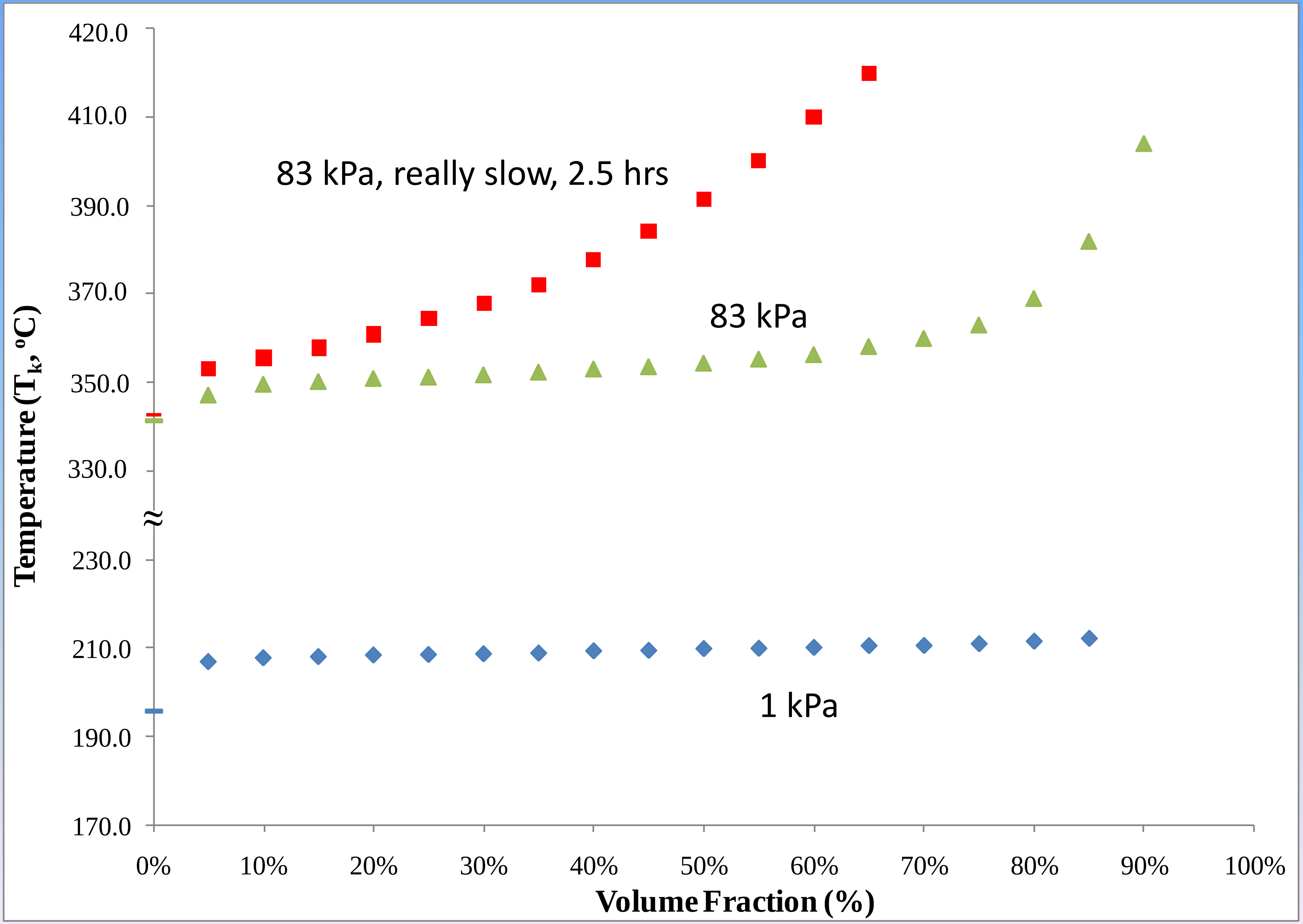


420.0
410.0
390.0
370.0
350.0
330.0
230.0
210.0
190.0
170.0
Temperature (T_k, °C)
83 kPa
1 kPa
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
Volume Fraction (%)


420.0
410.0
390.0
370.0
350.0
330.0
≈
230.0
210.0
190.0
170.0
Temperature (T_k, ºC)
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
Volume Fraction (%)
83 kPa
Slopes are the same
1 kPa



420.0
410.0
390.0
370.0
350.0
330.0
230.0
210.0
190.0
170.0
Temperature (T_k, °C)
83 kPa
Slopes are the same
No jump!
1 kPa
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
Volume Fraction (%)

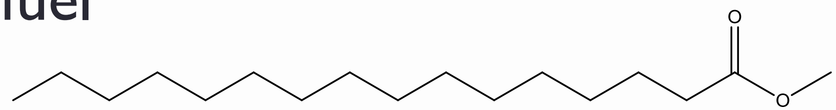


420.0
410.0
390.0
370.0
350.0
330.0
≈
230.0
210.0
190.0
170.0
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
Temperature (T_k, °C)
Volume Fraction (%)
83 kPa, really slow, 2.5 hrs
83 kPa
1 kPa

FAMEs

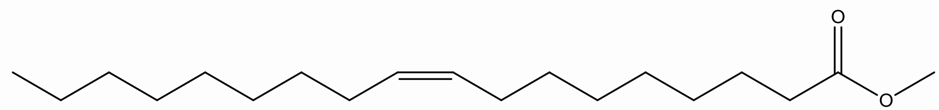
- Soybean-based biodiesel fuel

Soybean plant



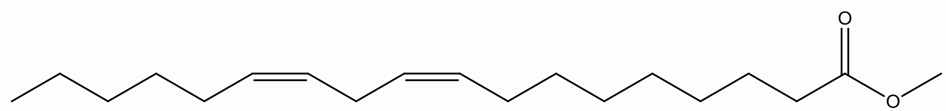
methyl palmitate

11 %



methyl oleate

24 %

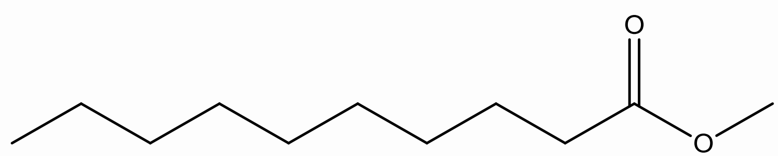


methyl linoleate

54 %

- Cuphea plant-based biodiesel fuel

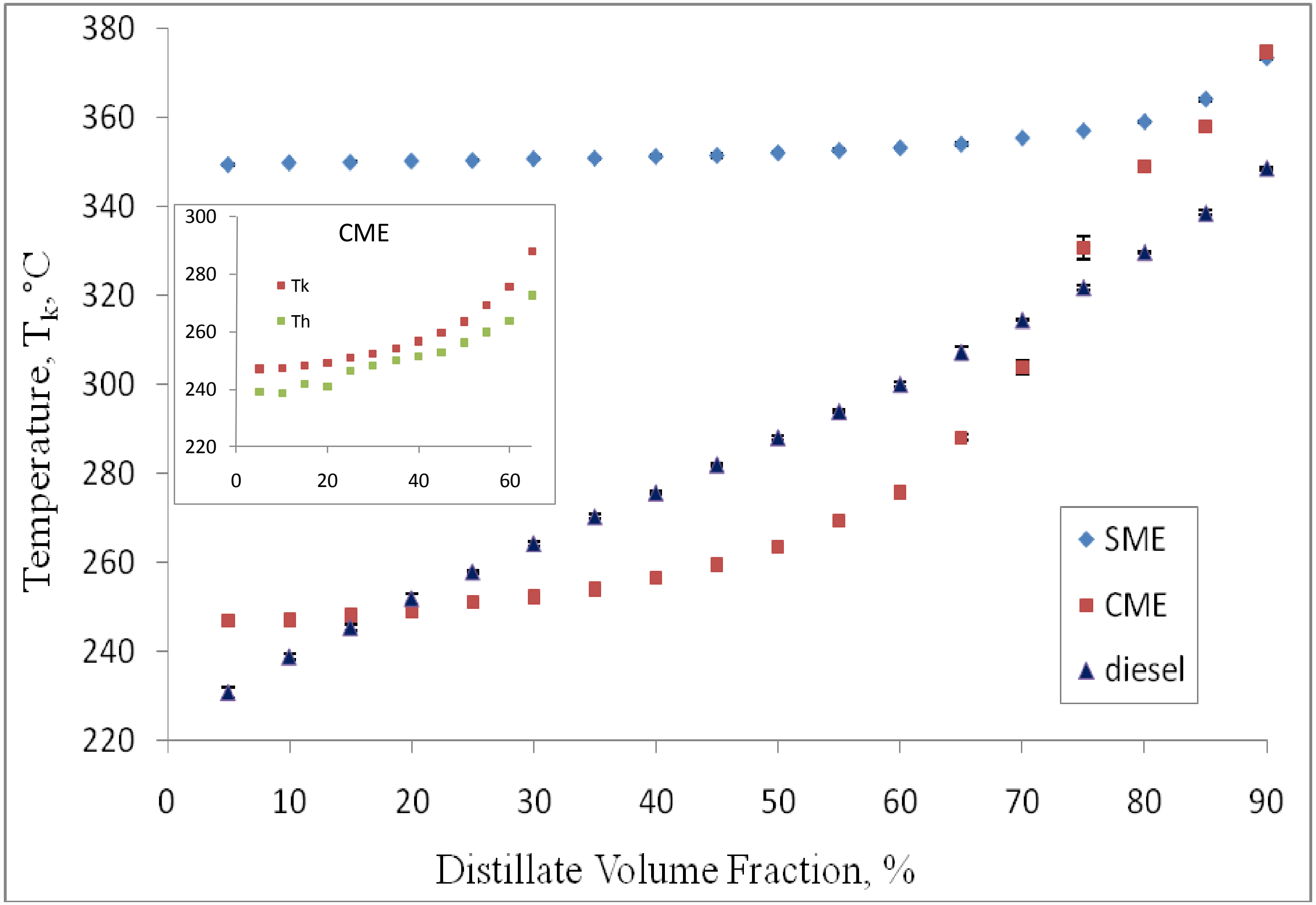
Cuphea plant



methyl decanoate

74 %

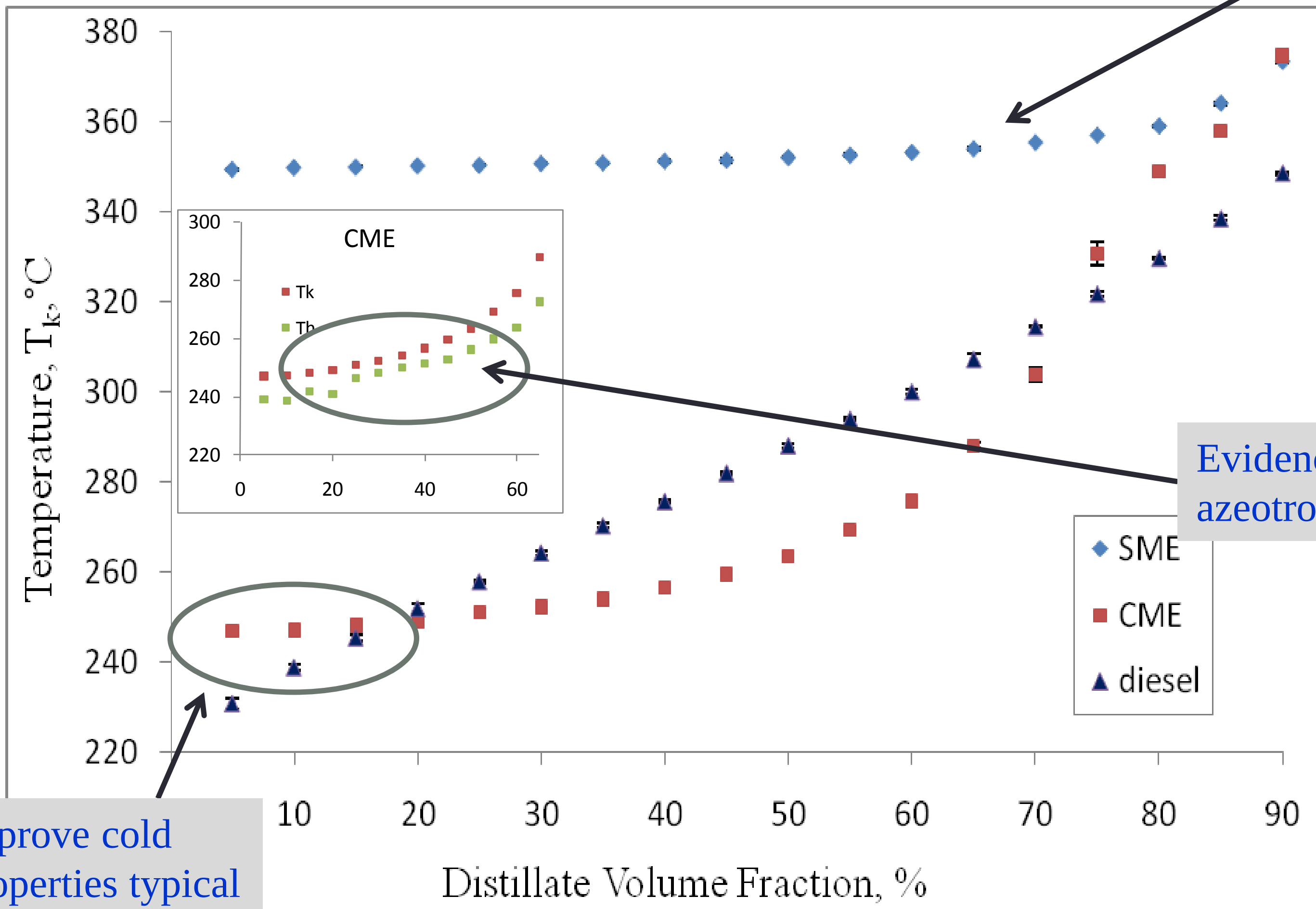
Distillation curves for cuphea (CME) vs. soy (SME) -based biodiesel fuels



- The temperature range from 5 % to 90 % distillate volume fraction for CME spans 130 °C, whereas for SME this temperature range spans only 25 °C.

Distillation curves for SME (Soy-based B100) compared to CME (cuphea-derived biodiesel fuel

Over 80 % C18 FAMES

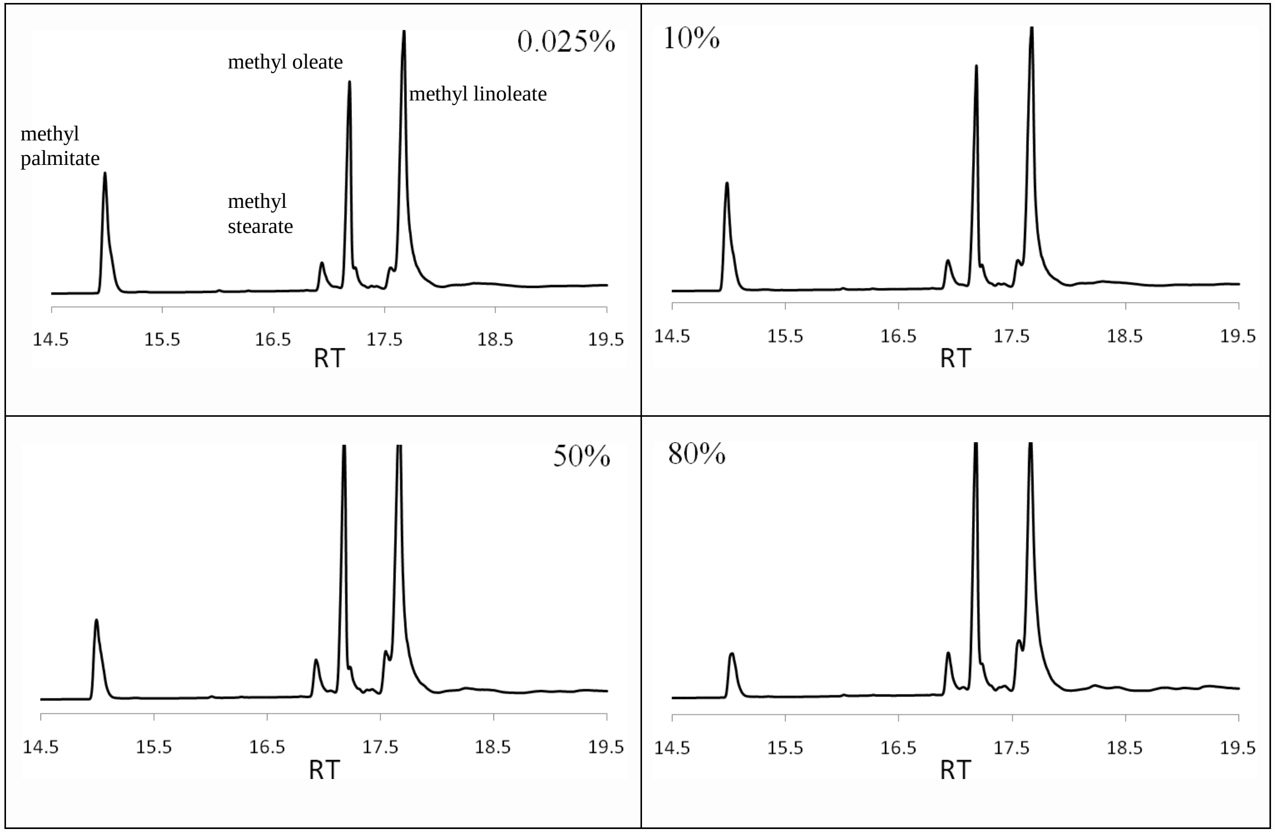


Evidence of possible azeotrope

May improve cold flow properties typical of soy-based biodiesel fuels

Chromatograms of four distillate volume fractions for soybean-based biodiesel fuel

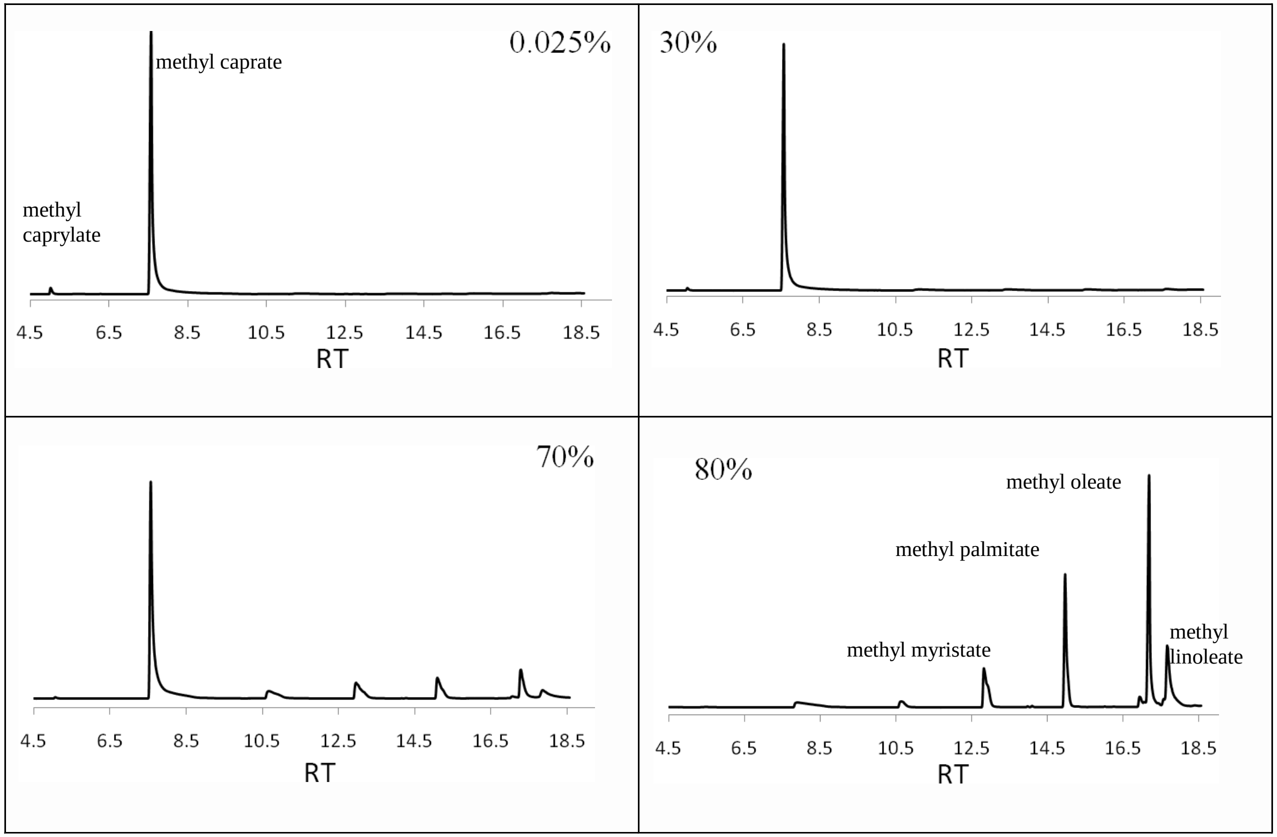
(a) SME Biodiesel Fuel



Soybean plant

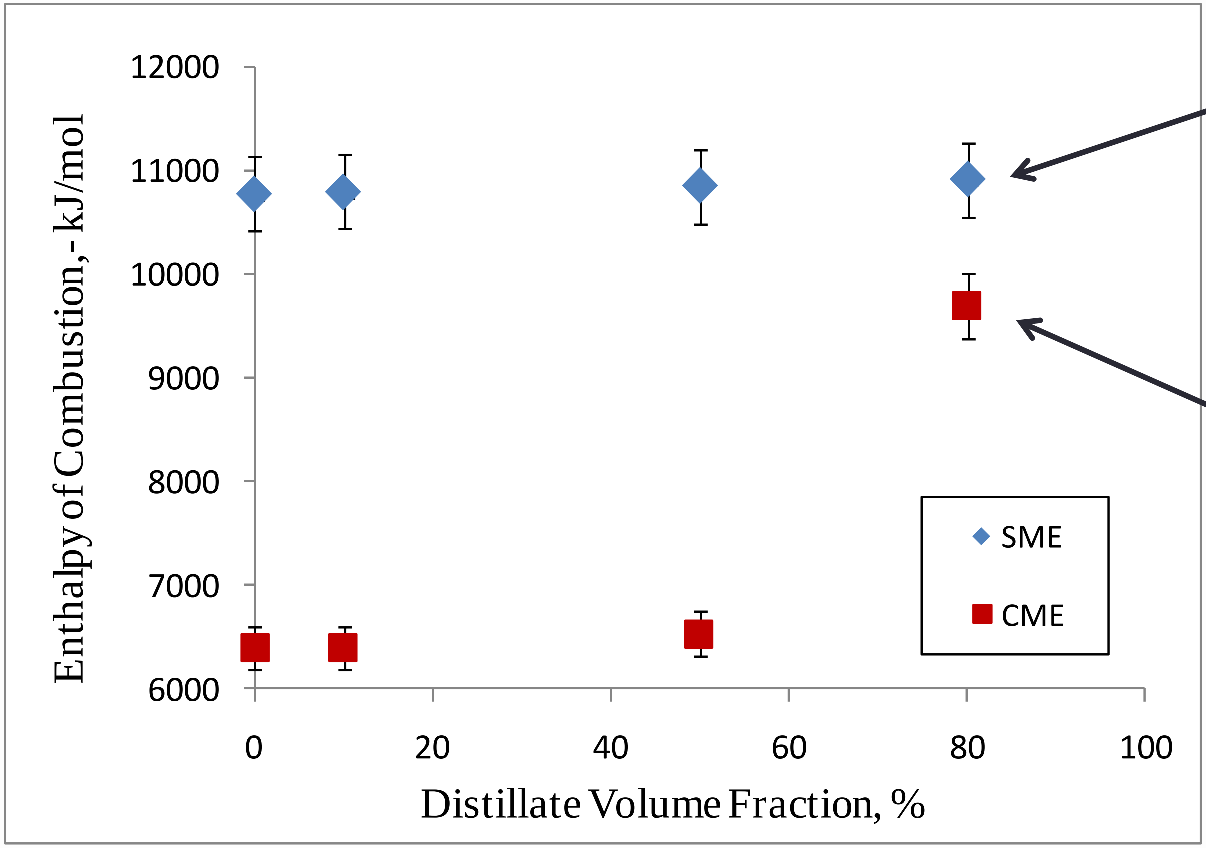
Chromatograms of four distillate volume fractions for cuphea-based biodiesel fuel

(b) CME Biodiesel Fuel



Cuphea plant

Composite enthalpy of combustion



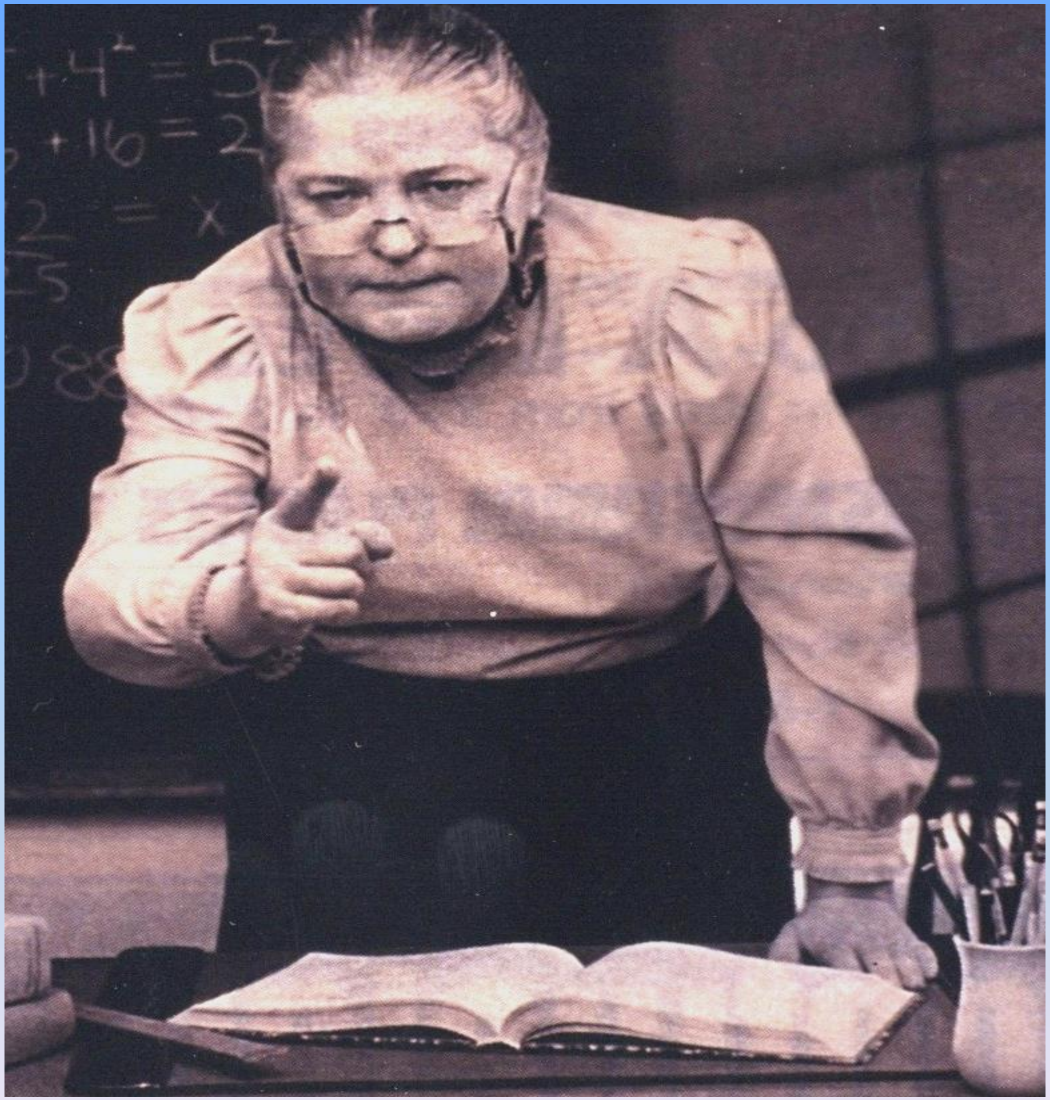
Soybean plant

Cuphea plant

- The enthalpy of combustion for the biodiesel fuels SME and CME presented at four distillate cuts, 0.025 % (the first drop), 10 %, 50 %, and 80 %.

Take Home Messages:

NOT:
you’re doing it wrong, do it my way



BUT RATHER:

The move to fundamental properties offer an alternative with **many powerful advantages**

3790 *Energy & Fuels* 2009, 23, 3790–3797

Model for the Thermodynamic Properties of a Biodiesel Fuel

Marcia L. Huber, Eric W. Lemmon, Andrei Kazakov, Lisa S. Ott,[†] and Thomas J. Bruno*

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We present an equation-of-state approach to modeling the thermodynamic properties of a biodiesel fuel. Preliminary Helmholtz-type equations of state were developed with limited experimental data for five fatty acid methyl esters (FAMEs) that are the primary constituents of soy-based biodiesel fuel, namely, methyl palmitate, methyl stearate, methyl oleate, methyl linoleate, and methyl linolenate. These components were combined in a mixture model using ideal mixing to represent the thermodynamic properties of a biodiesel fuel. We performed limited experimental measurements on the density, sound speed, and initial boiling point of two biodiesel fuel samples and compared the results with the model.

Introduction

Biodiesel fuel is a renewable fuel comprised of monoalkyl esters of long chain fatty acids. It can be produced from a variety of feedstocks including common vegetable oils (soybean, cottonseed, palm, peanut, canola, sunflower, safflower, coconut), animal fats (tallow), and even waste cooking oil.[1] In the United

For biodiesel fuel to replace or extend petroleum-derived diesel fuel on a large scale, it is necessary to be able to substitute the two fuels in a fairly straightforward manner (that is, biodiesel fuel, or mixtures thereof, should ideally be drop-in replacements). As the market accepts the various blends of biodiesel fuel mentioned above, the availability of thermophysical property information will become more critical. It is impracti-

Helmholtz Equation of State

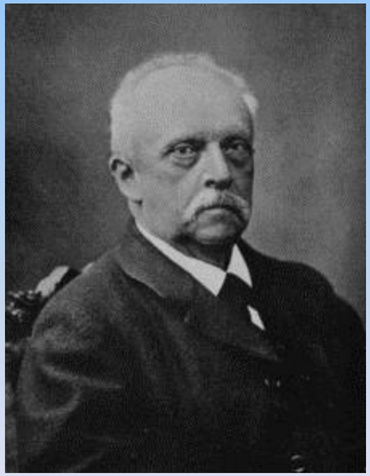
- Formulated in terms of $a(T, \rho)$ instead of $p(T, \rho)$

$$a(\rho,T) = a^0(\rho,T) + a^r(\rho,T)$$

ideal gas contribution — residual contribution

- All single phase properties can be calculated as derivatives of the Helmholtz energy

$$p = \rho^2 \left(\frac{\partial a}{\partial \rho}\right)_T$$



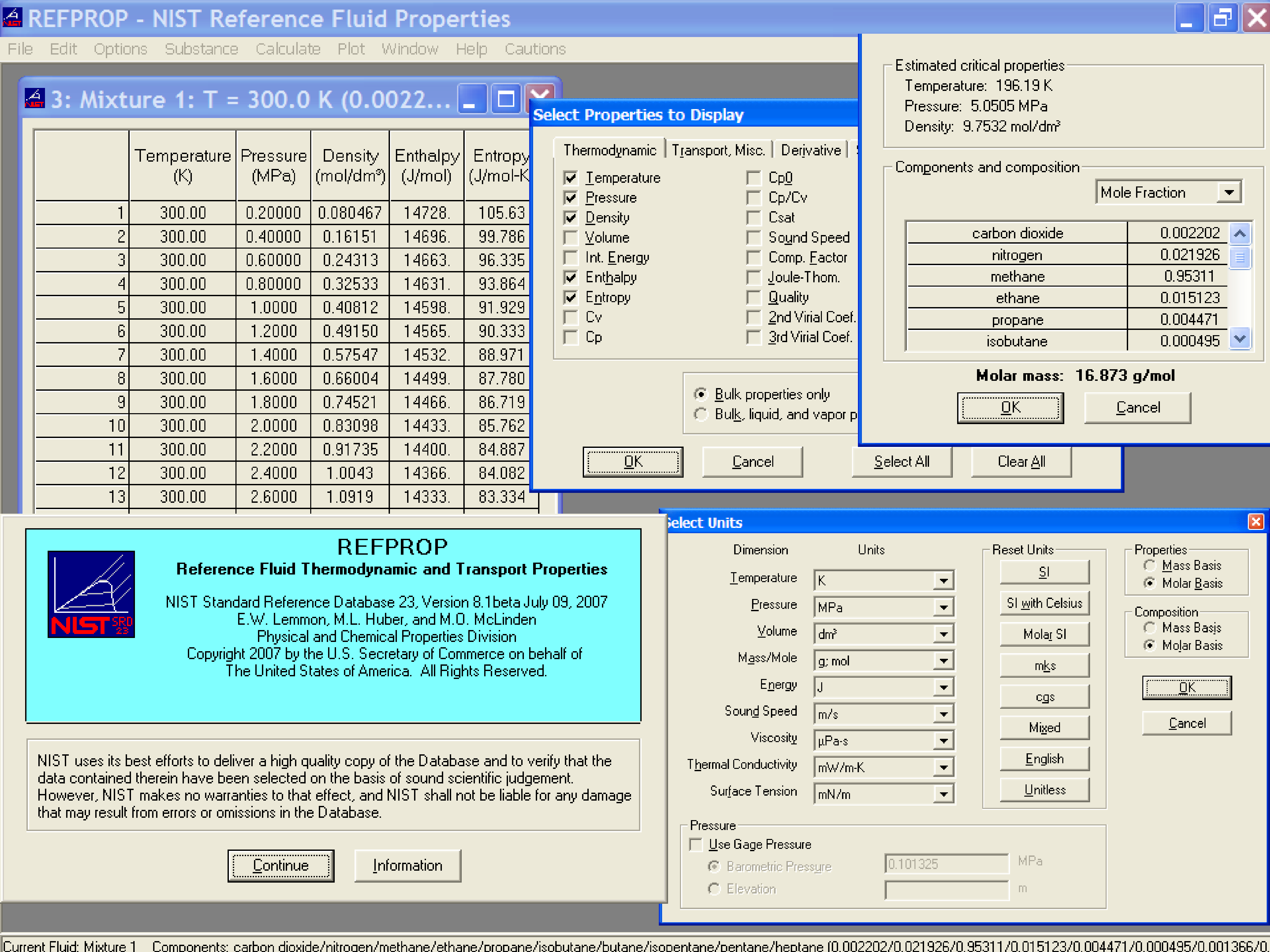
Old Man Helmholtz

- Typical form of residual contribution

$$\alpha^r(\delta,\tau) = \frac{a^r}{RT} = \sum N_k \delta^{d_k} \tau^{t_k} + \sum N_k \delta^{d_k} \tau^{t_k} e^{-\delta^{l_k}}$$

summations typically have 4-20 terms

$$\delta = \frac{\rho}{\rho_c} \qquad \tau = \frac{T_c}{T}$$


REFPROP - NIST Reference Fluid Properties
File Edit Options Substance Calculate Plot Window Help Cautions
3: Mixture 1: T = 300.0 K (0.0022...
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1 300.00 0.20000 0.080467 14728. 105.63
2 300.00 0.40000 0.16151 14696. 99.786
3 300.00 0.60000 0.24313 14663. 96.335
4 300.00 0.80000 0.32533 14631. 93.864
5 300.00 1.0000 0.40812 14598. 91.929
6 300.00 1.2000 0.49150 14565. 90.333
7 300.00 1.4000 0.57547 14532. 88.971
8 300.00 1.6000 0.66004 14499. 87.780
9 300.00 1.8000 0.74521 14466. 86.719
10 300.00 2.0000 0.83098 14433. 85.762
11 300.00 2.2000 0.91735 14400. 84.887
12 300.00 2.4000 1.0043 14366. 84.082
13 300.00 2.6000 1.0919 14333. 83.334
Select Properties to Display
Thermodynamic | Transport, Misc. | Derivative
Temperature Pressure Density Volume Int. Energy Enthalpy Entropy Cv Cp
Cp0 Cp/Cv Csat Sound Speed Comp. Factor Joule-Thom. Quality 2nd Virial Coef. 3rd Virial Coef.
Bulk properties only
Bulk, liquid, and vapor p
OK Cancel Select All Clear All
Estimated critical properties
Temperature: 196.19 K
Pressure: 5.0505 MPa
Density: 9.7532 mol/dm³
Components and composition
Mole Fraction
carbon dioxide 0.002202
nitrogen 0.021926
methane 0.95311
ethane 0.015123
propane 0.004471
isobutane 0.000495
Molar mass: 16.873 g/mol
OK Cancel
REFPROP
Reference Fluid Thermodynamic and Transport Properties
NIST Standard Reference Database 23, Version 8.1beta July 09, 2007
E.W. Lemmon, M.L. Huber, and M.O. McLinden
Physical and Chemical Properties Division
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Current Fluid: Mixture 1 Components: carbon dioxide/nitrogen/methane/ethane/propane/isobutane/butane/isopentane/pentane/heptane (0.002202/0.021926/0.95311/0.015123/0.004471/0.000495/0.001366/0.

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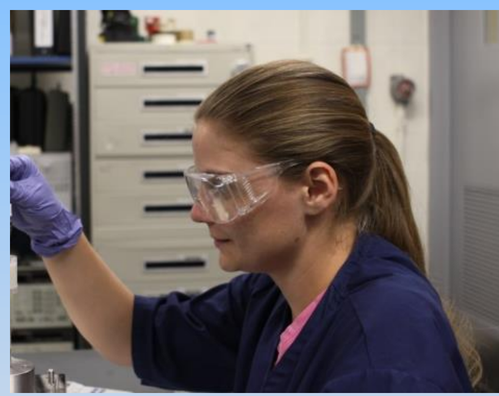

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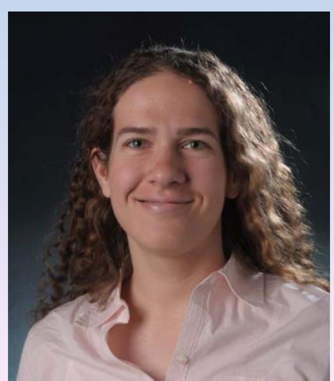

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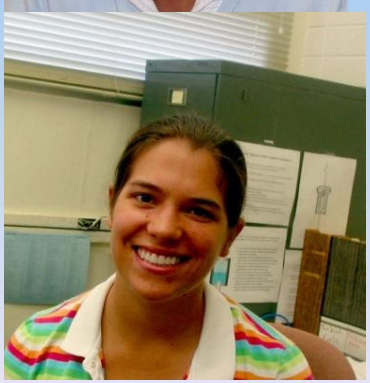

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