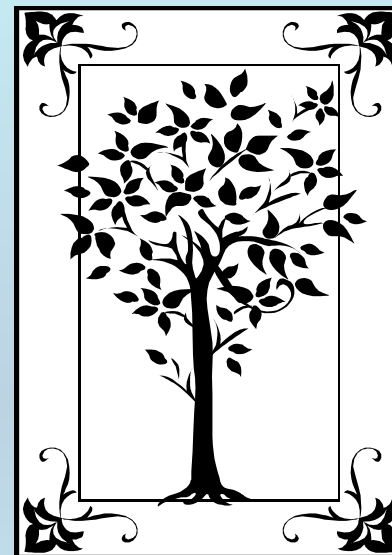


**METADATA AND NUMERICAL DATA CAPTURE:
Critical Properties
(2 – Components)**

***Guided Data*
Capture (GDC)**



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Critical Properties**
(2-components)
with the **Guided Data Capture (GDC)** software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. **It is not necessary to enter *all* compounds before entering *all* samples, etc.**

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

Gas–Liquid Critical Properties of Ethylene + Benzene

Tao Liu,[†] Jin-Yan Fu,[‡] Kun Wang,[‡] Yong Gao,[†] and Wei-Kang Yuan^{*,†}

UNILAB Research Center of Chemical Reaction Engineering, and Thermodynamics Research Laboratory, East China University of Science and Technology, Shanghai 200237, People's Republic of China

Gas–liquid critical properties of ethylene + benzene have been measured over the whole composition range by using a high-pressure view cell with direct visual observation. The critical points of the two pure components are in good agreement with literature values. Critical lines show the expected type I fluid phase behavior. Our results are compared with those of Lyubetski,¹ who obtained critical property values through extrapolation of vapor–liquid-phase equilibrium data. Using the Peng–Robinson equation of state, the binary interaction parameter k_B , obtained from vapor–liquid equilibrium data at 348.15 K,² was used to calculate the critical temperature and the critical pressure. The agreement between our experimental values and the calculated values is satisfactory.

Critical Properties for Ethylene + Benzene at various compositions

This data set is
considered here.



Table 2. Critical Properties of Ethylene (1) + Benzene (2)

| x_1 | T_c/K | P_c/MPa | $\rho_c/\text{g}\cdot\text{cm}^{-3}$ |
|-------|----------------|------------------|--------------------------------------|
| 1.000 | 282.75 | 5.07 | 0.210 |
| 0.911 | 331.25 | 8.43 | 0.304 |
| 0.831 | 372.47 | 10.78 | 0.352 |
| 0.700 | 438.25 | 11.53 | 0.379 |
| 0.600 | 461.21 | 10.97 | 0.380 |
| 0.500 | 488.25 | 9.93 | 0.378 |
| 0.402 | 511.85 | 9.15 | 0.370 |
| 0.300 | 528.25 | 7.72 | 0.348 |
| 0.197 | 542.65 | 6.71 | 0.340 |
| 0.100 | 552.75 | 6.06 | 0.318 |
| 0.000 | 563.65 | 5.01 | 0.297 |

NOTE: The T_c values will be captured in this example. The p_c and ρ_c values are captured independently in a completely analogous manner.

Experimental Method Info:

Experimental Setup. Critical point measurements were conducted using a high-pressure view cell. The cell can be operated at temperatures up to 623 K and pressures up to 13 MPa.

Uncertainty Info:

The cell was placed in an air thermostat, whose temperature was controlled at an accuracy of ± 0.2 K

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction **Property** Data Tables

2001 liu fu 0

- benzene
 - Sample 1 (cm,99.5m%,nc,y;)
- ethylene
 - Sample 1 (cm,99.9m%,nc;)
- benzene + ethylene**

2. **CLICK**
Property

1. **SELECT** the *mixture* for which the data are to be captured.

NOTE: The **bibliographic information, compound identities, sample descriptions,** and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)

Property and experimental method for benzene + ethylene

Help

Property group: Critical properties

Property: Critical temperature

Units: K

Method of measurement:

Experimental purpose:

Comment (optional)

Property as function of state variable(s)

Invariant Property (No state variables)

Cancel

1. SELECT the **Property Group:**
Critical properties from the menu.

2. SELECT the **Property:**
Critical Temperature.

3. SELECT the **Units; K.**

1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

Units: K

Method of measurement: Visual observation in a stirred cell

Details...

Experimental purpose: Principal objective of the work

2. SELECT the **Experimental Purpose** from the list provided.

Comment (optional)

Property as function of state variable(s)

Invariant Property (No state variables)

3. CLICK *Property as function of state variable(s)*

Cancel

Experiment details

Select the statements, which are true for the reported measurement

Mercury-in-glass thermometer used
Dissolved air not removed
Compound is unstable

Accept

When the Method is chosen, a second form might appear. This form is used to provide some additional information concerning the Method.

SELECT those that apply and *CLICK Accept.*

NOTE: These fields are filled automatically based on the property.

Critical temperature (K) as function of 1 variable(s)

Mixture: benzene + ethylene

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set #: 1 Sample #: 1 Sample #: 1

Phase of the Property Value(s): Liquid

Phase 2: Gas

Constraint 1 (Fixed value of): Liquid-gas critical state

Independent variable 1: Mole fraction of ethylene of Liquid Units: Dimensionless Uncertainty: %

Definition of Measurement Results (Absolute vs Relative): Direct value

Data presentation: Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Critical temperature (K) as function of 1 variable(s)

Mixture: benzene + ethylene

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set # 1

Phase of the Property Value(s) Liquid Precision of the Property Value(s) 0.2 K

Phase 2 Gas

Constraint 1 (Fit) Liquid-gas critical

Independent variable Mole fraction of benzene

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Multiple *samples* for a given component can be accommodated, but this is rarely needed.

1. SELECT the **Independent Variable**
(*Mole fraction of ethylene*, here) from the menus.

Mixture: benzene + ethylene

Phases in equilibrium: 2 Constraints: 1 Independent variables: 1 Property set # 1 Sample # 1 Sample # 1

Phase of the Property Value(s) Liquid

Phase 2 Gas

Constraint 1 (Fixed value of) Liquid-gas critical state

Independent variable 1 Mole fraction of ethylene or Liquid

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental value

Comments (Optional):

Property and method Numerical Data Cancel

2. SELECT **Units for the **Variable**.**
Include **Uncertainties, if known.**

3. CLICK *Numerical Data*

TYPE, or much preferably,
PASTE the variable and
property values into the table.
See next page...

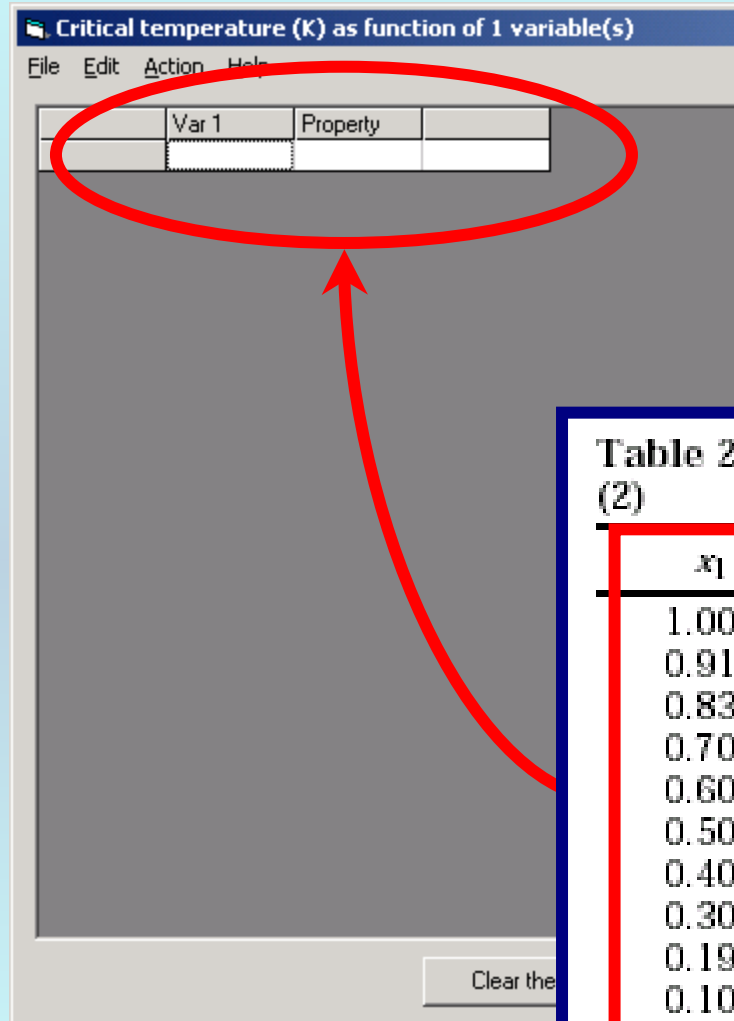


Table 2. Critical Properties of Ethylene (1) + Benzene (2)

| x_1 | T_c/K | P_c/MPa | $\rho_c/g\cdot cm^{-3}$ |
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| 0.700 | 438.25 | 11.53 | 0.379 |
| 0.600 | 461.21 | 10.97 | 0.380 |
| 0.500 | 488.25 | 9.93 | 0.378 |
| 0.402 | 511.85 | 9.15 | 0.370 |
| 0.300 | 528.25 | 7.72 | 0.348 |
| 0.197 | 542.65 | 6.71 | 0.340 |
| 0.100 | 552.75 | 6.06 | 0.318 |
| 0.000 | 563.65 | 5.01 | 0.297 |

Critical temperature (K) as function of 1 variable(s)

File Edit Action Help

| | Var 1 | Property |
|----|-------|----------|
| 1 | 1.000 | 282.75 |
| 2 | 0.911 | 331.25 |
| 3 | 0.831 | 372.47 |
| 4 | 0.700 | 438.25 |
| 5 | 0.600 | 461.21 |
| 6 | 0.500 | 488.25 |
| 7 | 0.402 | 511.85 |
| 8 | 0.300 | 528.25 |
| 9 | 0.197 | 542.65 |
| 10 | 0.100 | 552.75 |
| 11 | 0.000 | 563.65 |

Clear the Table

Table 2. Critical Properties of Ethylene (1) + Benzene (2)

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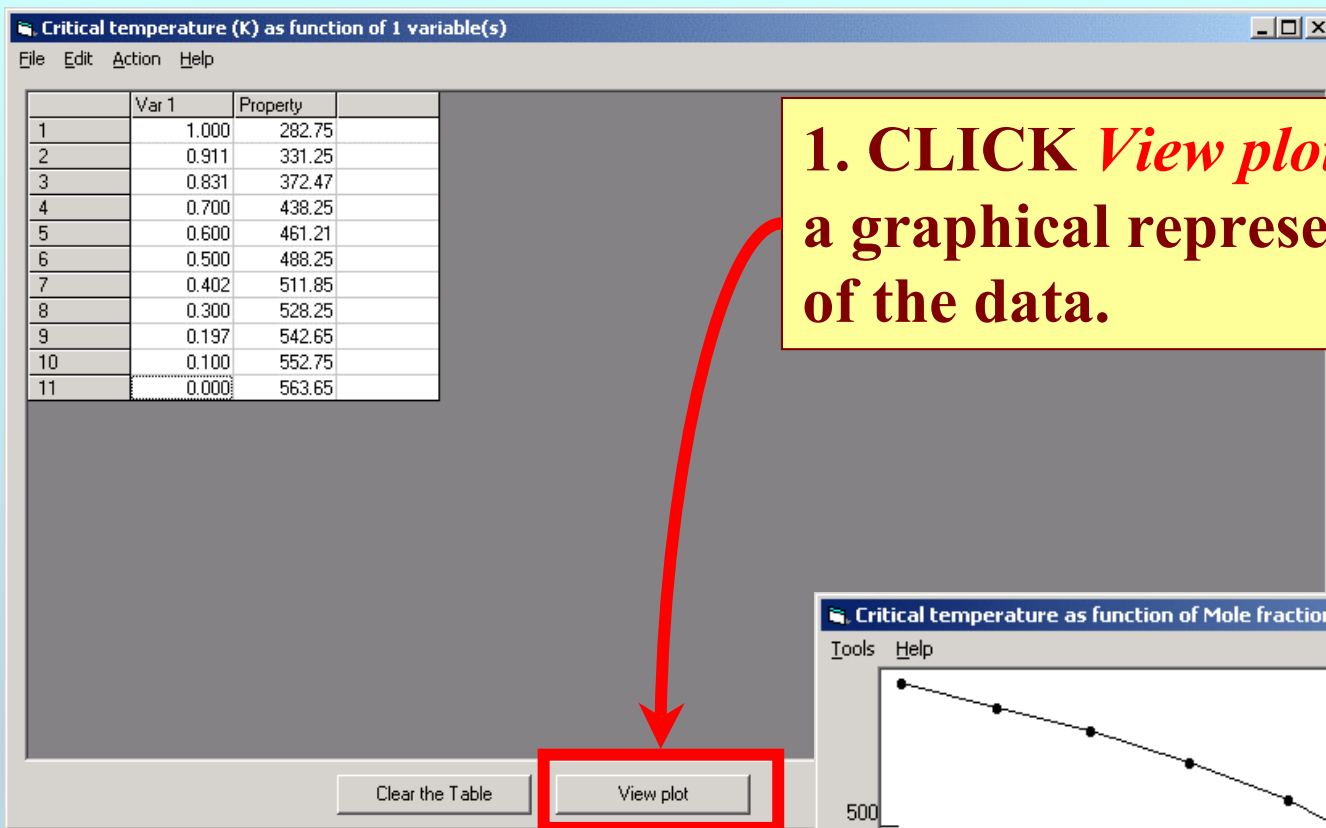
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

Critical temperature (K) as function of 1 variable(s)

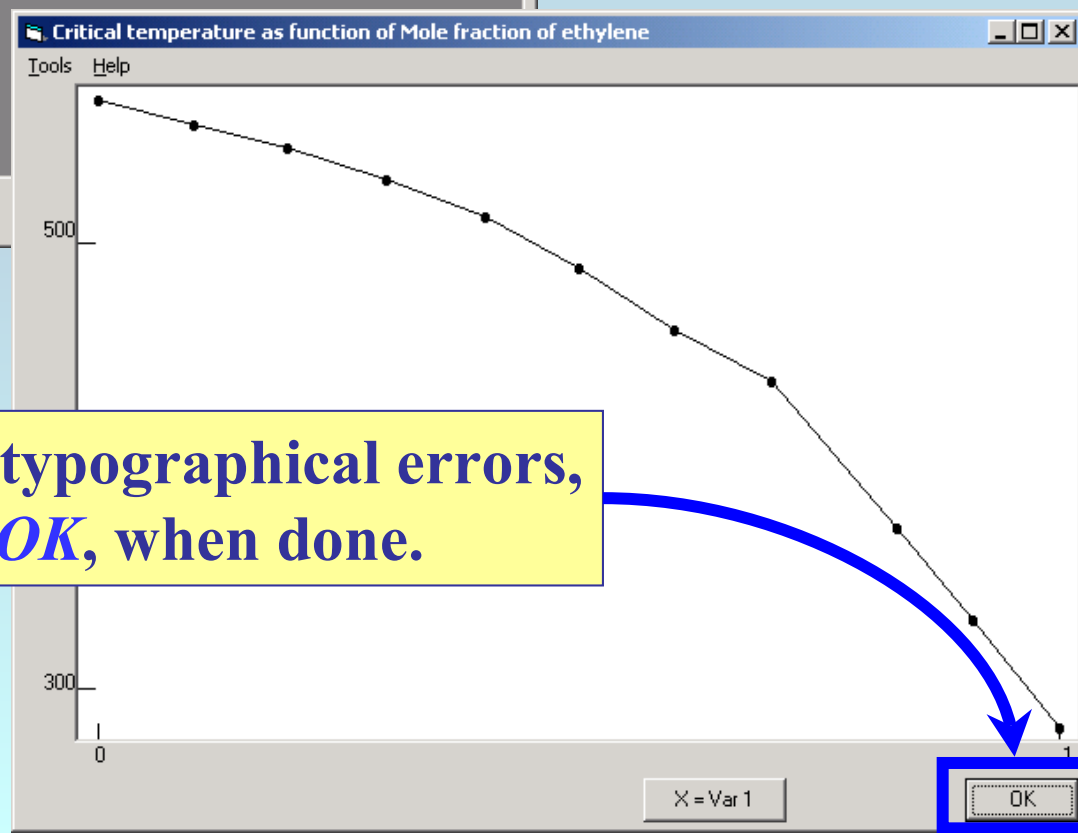
File Edit Action Help

| | Var 1 | Property |
|----|-------|----------|
| 1 | 1.000 | 282.75 |
| 2 | 0.911 | 331.25 |
| 3 | 0.831 | 372.47 |
| 4 | 0.700 | 438.25 |
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| 8 | 0.300 | 528.25 |
| 9 | 0.197 | 542.65 |
| 10 | 0.100 | 552.75 |
| 11 | 0.000 | 563.65 |

Clear the Table View plot



1. CLICK *View plot* to see a graphical representation of the data.



3. Check for typographical errors, and CLICK *OK*, when done.

Critical temperature (K) as function of 1 variable(s)

File Edit Action Help

| | Var 1 | Property |
|----|-------|----------|
| 1 | 1.000 | 282.75 |
| 2 | 0.911 | 331.25 |
| 3 | 0.831 | 372.47 |
| 4 | 0.700 | 438.25 |
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| 8 | 0.300 | 528.25 |
| 9 | 0.197 | 542.65 |
| 10 | 0.100 | 552.75 |
| 11 | 0.000 | 563.65 |

CLICK *Accept*

Clear the Table View plot **Accept** Cancel

Guided Data Capture - Thermophysical and Thermochemical

File Edit Tools Help

Reference

Compound

Sample

Mixture

[-] 2001 liu fu 0

[-] benzene

... Sample 1 (cm,99.5m%,no)

[-] ethylene

... Sample 1 (cm,99.9m%,no:)

[-] benzene + ethylene

^1: TC (Set 1), B Method:VISOBSS dTC=0.2

NOTE: The new data set now appears in the navigation tree under the appropriate *mixture*.

NOTE: DOUBLE CLICKING on the *data set* allows editing of all entered information.

END

**Continue with other compounds,
samples, properties, reactions, etc...**

or save your file and exit the program.