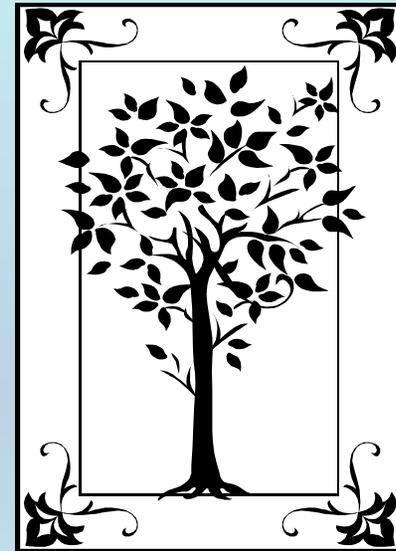


**METADATA AND NUMERICAL DATA CAPTURE:  
Liquid-Liquid Equilibria  
(3-Component: Binodal Curve)**

**Guided Data  
Capture (GDC)**



This tutorial describes  
**METADATA AND NUMERICAL DATA CAPTURE:**  
for **Liquid-Liquid Equilibria (3 components)**  
**BINODAL CURVE**  
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:

1452

*J. Chem. Eng. Data* 2001, 46, 1452–1456

## **Liquid–Liquid Equilibria of the System Water + Acetic Acid + 2-Hexanone at 25 °C and 35 °C**

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Liquid–liquid equilibria of the system water + acetic acid + 2-hexanone at 25 °C and 35 °C were studied to evaluate 2-hexanone as an extraction agent in aqueous solutions of acetic acid. The experimental data were fitted using the NRTL and UNIQUAC equations. Equilibrium predictions, applying the UNIFAC method, were also made with the use of liquid–liquid equilibrium specific parameters for both temperatures.

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## Binodal Curve data for (water + ethanol + dimethylphthalate) at $T = 298.15$ K and $p = 101.3$ kPa

Table 2. Binodal Curve Mole Fractions for the Systems  
Water (1) + Ethanol (2) + Dialkyl Phthalate (3) at  
298.15 K

$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
Water (1) + Ethanol (2) + Dimethyl Phthalate (3)					
0.4211	0.2589	0.3200	0.6052	0.2650	0.1298
0.4831	0.2766	0.2403	0.6699	0.2508	0.0793
0.5132	0.2857	0.2012	0.7218	0.2266	0.0516
0.5839	0.2710	0.1451	0.7246	0.2247	0.0507
0.6044	0.2650	0.1306	0.7606	0.2064	0.0329
Water (1) + Ethanol (2) + Diethyl Phthalate (3)					
0.4117	0.3840	0.2043	0.5997	0.3298	0.0705
0.4890	0.3706	0.1404	0.6759	0.2865	0.0376
0.5277	0.3569	0.1154	0.6858	0.2808	0.0334
0.5812	0.3370	0.0818	0.6931	0.2765	0.0304
Water (1) + Ethanol (2) + Dibutyl Phthalate (3)					
0.2806	0.4747	0.2447	0.4348	0.4845	0.0807
0.3323	0.4903	0.1774	0.4539	0.4728	0.0733
0.3738	0.4732	0.1530	0.4660	0.4699	0.0641
0.4062	0.4893	0.1045	0.4779	0.4669	0.0552
0.4249	0.4769	0.0982	0.4862	0.4661	0.0477

## Experimental Method Info:

The first step to determining the liquid + liquid equilibrium was establishing the binodal curve in the critical region using the turbidimetry titration method. Homoge-

This data set is considered here.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

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

- 2002 ben reh 0
  - dimethyl phthalate
    - Sample 1 (cm,99.0m%,nc;:)
  - diethyl phthalate
    - Sample 1 (cm,99.0m%,nc;se;)
  - dibutyl phthalate
    - Sample 1 (cm,99.0m%,nc;se;)
  - water
    - Sample 1 (cm;(Deionized with Milli-Q RG system);99.9m%,est)
  - ethanol
    - Sample 1 (cm,99.9m%,nc;:)
  - ethanol + dimethyl phthalate + water**

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 related to capture of this information.)

Property and experimental method for ethanol + dimethyl phthalate + water

Help

Property group:

Property:

Units:

Method of measurement:

Experimental purpose:

Comment (optional)

Cancel

**SELECT the *Property Group - Composition at phase equilibrium***

- Critical properties
- Vapor pressure; Boiling temperature; and Azeotropic T & P
- Phase transition properties
- Composition at phase equilibrium
- Activity; Fugacity; and Osmotic properties
- Volumetric properties
- Heat capacity and derived properties
- Excess; partial; and apparent energetic properties

Property and experimental method for ethanol + dimethyl phthalate + water

Help

Property group: Composition at phase equilibrium

Property: MolarRity of water  
Mole fraction of ethanol  
Mole fraction of dimethyl phthalate  
Mole fraction of water

Units:

Method of measurement:

Experimental purpose:

**SELECT** the composition (*mole fraction* here) of one component (*ethanol* here) to serve as the *Property*. The component selection is arbitrary.

Table 2. Binodal Curve Mole Fractions for the Systems Water (1) + Ethanol (2) + Dialkyl Phthalate (3) at 298.15 K

$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
Water (1) + Ethanol (2) + Dimethyl Phthalate (3)					
0.4211	0.2589	0.3200	0.6052	0.2650	0.1298
0.4831	0.2766	0.2403	0.6699	0.2508	0.0793
0.5132	0.2857	0.2012	0.7218	0.2266	0.0516
0.5839	0.2710	0.1451	0.7246	0.2247	0.0507
0.6044	0.2650	0.1306	0.7606	0.2064	0.0329

Cancel

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

The first step to determining the liquid + liquid equilibrium was establishing the binodal curve in the critical region using the turbidimetry titration method. Homoge-

Method of measurement: Titration method

Experimental purpose: Principal objective of the work

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

Comment (optional)

OK

Cancel

3. CLICK *OK*

# SELECTION of # of Phases in Equilibrium and # of Constraints

Mole fraction of ethanol () (Dimensionless) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Phase of the Property Value(s) Precision of the Property Value(s)  Dimensionless  %

Comments (Optional):

Property and method Numerical Data Cancel

**Enter the # of phases in equilibrium.**

There are **2** phases (liquids) in equilibrium in the case of a *Binodal Curve*.

**Enter the # of Constraints.**

There are **2** constraints in the present example; *temperature and pressure*.

Mole fraction of ethanol () (Dimensionless) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Sample # 1 Sample # 1 Sample # 1

Phase of the Property Value(s)

Dimensionless

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

Independent variable 1

Units: Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)

Data presentation

Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

Mole fraction of ethanol () (Dimensionless) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Phase of the Property Value(s)

- Liquid of pure ethanol
- Liquid of pure dimethyl phthalate
- Liquid of pure water
- Liquid mixture 1
- Liquid mixture 2
- Liquid mixture 3
- Fluid (supercritical or subcritical phases)
- Gas

Precision of the Property Value(s)  
 Dimensionless  %

Independent variable 1

Definition of M

Data presentation  
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

**SELECT *Liquid Mixture 1* from the list provided for the Phase of the Property value.**

**All associated fields appear automatically.**

Mole fraction of ethanol (Liquid mixture 1) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Phase of the Property Value(s) Liquid mixture 1 Precision of the Property Value(s)   Dimensionless  %

Phase 2  
Liquid mixture 2

Constraint 1 (Fixed value of)  of Liquid mixture 1 Units:  Uncertainty:

Constraint 2 (Fixed value of)  of Liquid mixture 1 Units:  Uncertainty:

Independent variable 1  Units:  Uncertainty:   %

Definition of Measurement Results (Absolute)

Data presentation  
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

**SELECT *Liquid Mixture 2* for Phase 2**

# Specification of constraints, constraint values, and constraint units

Mole fraction of ethanol (Liquid mixture 1) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Phase of the Property Value(s) Liquid mixture 1 Precision of the Property Value(s)   Dimensionless  %

Phase 2 Liquid mixture 2

Constraint 1 (Fixed value of) Temperature of Liquid mixture 1 Value: 298.15 Units: K Uncertainty:  %

Constraint 2 (Fixed value of) Pressure of Liquid mixture 1 Value: 101 Units: kPa Uncertainty:  %

Independent variable 1 of Liquid mixture 1 Units:  Uncertainty:  %

Definition of Measurement Results (Absolute vs Relative)

Property and method

**1. SELECT *Constraint 1* and *Constraint 2* from the lists provided (*T* and *p* here).**

**2. TYPE *Values* and SELECT *Units* for each Constraint. Include *Uncertainties*, if known.**

# SELECTION of the Independent Variable

Mole fraction of ethanol (Liquid mixture 1) as function of 1 variable(s)

Mixture: ethanol + dimethyl phthalate + water

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

Phase of the Property Value(s) Liquid mixture 1 Precision of the Property Value(s)   Dimensionless  %

Phase 2 Liquid mixture 2

Constraint 1 (Fixed value of) Temperature of Liquid mixture 1 Value: 298.15 Units: K Uncertainty:  %

Constraint 2 (Fixed value of) Pressure of Liquid mixture 1 Value: 101 Units: kPa Uncertainty:  %

Independent variable 1

Temperature  
Pressure  
Partial pressure of ethanol  
Partial pressure of dimethyl phthalate  
Partial pressure of water  
Mole fraction of ethanol  
Mole fraction of dimethyl phthalate  
Mole fraction of water

Comments (Optional):

**SELECT** the composition (*mole fraction* here) of one of the other components (*water* here) as the **Independent Variable**.

# Measurement definition and Data presentation

Mole fraction of ethanol (Liquid mixture 1) as function of

Mixture: ethanol + dimethyl phthalate + water

Phases in equilibrium: 2 Constraints: 2 Independent v

Phase of the Property Value(s) Liquid mixture 1

Phase 2  
Liquid mixture 2

Constraint 1 (Fixed value of)  
Temperature of Liquid mixture 1 Value: 298.15 Units: K Uncertainty: %

Constraint 2 (Fixed value of)  
Pressure of Liquid mixture 1 Value: 101 Units: kPa Uncertainty: %

Independent variable 1  
Mole fraction of water of Liquid mixture 1

Definition of Measurement Results (Absolute vs Relative)  
Direct value

Data presentation  
Experimental values

Comments (Optional):

Property and method Numerical Data Cancel

1. SELECT *Direct Value* (as compared with *Relative Value*) from the list defining the **Measurement Results**

2. SELECT the appropriate **Data presentation** method. *Experimental values* here.

3. CLICK *Numerical Data*

Table 2. Binodal Curve Mole Fractions for the Systems Water (1) + Ethanol (2) + Dialkyl Phthalate (3) at 298.15 K

$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
Water (1) + Ethanol (2) + Dimethyl Phthalate (3)					
0.4211	0.2589	0.3200	0.6052	0.2650	0.1298
0.4831	0.2766	0.2403	0.6699	0.2508	0.0793
0.5132	0.2857	0.2012	0.7218	0.2266	0.0516
0.5839	0.2710	0.1451	0.7246	0.2247	0.0507
0.6044	0.2650	0.1306	0.7606	0.2064	0.0329

Mole fraction of ethanol (Dimensionless) as function

File Edit Action Help

	Var 1	Property
1	0.4211	0.2589
2	0.4831	0.2766
3	0.5132	0.2857
4	0.5839	0.2710
5	0.6044	0.2650
6	0.6052	0.2650
7	0.6699	0.2508
8	0.7218	0.2266
9	0.7246	0.2247
10	0.7606	0.2064

Clear the Table View plot Accept Cancel

**TYPE, or much preferably, PASTE the variable and property values into the table.**

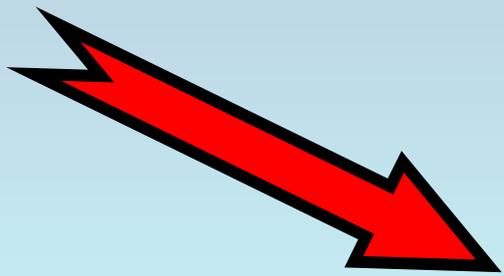
Mole fraction of ethanol (Dimensionless) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.4211	0.2589
2	0.4831	0.2766
3	0.5132	0.2857
4	0.5839	0.2710
5	0.6044	0.2650
6	0.6052	0.2650
7	0.6699	0.2508
8	0.7218	0.2266
9	0.7246	0.2247
10	0.7606	0.2064

Clear the Table View plot

**1. CLICK *View plot* to see a plot and check for typographical errors.**



Mole fraction of ethanol as function of Mole fraction of water

Tools Help

Mole fraction of water (X = Var 1)	Mole fraction of ethanol (Property)
0.4211	0.2589
0.4831	0.2766
0.5132	0.2857
0.5839	0.2710
0.6044	0.2650
0.6052	0.2650
0.6699	0.2508
0.7218	0.2266
0.7246	0.2247
0.7606	0.2064

X = Var 1 OK

**2. CLICK *OK*, when done**

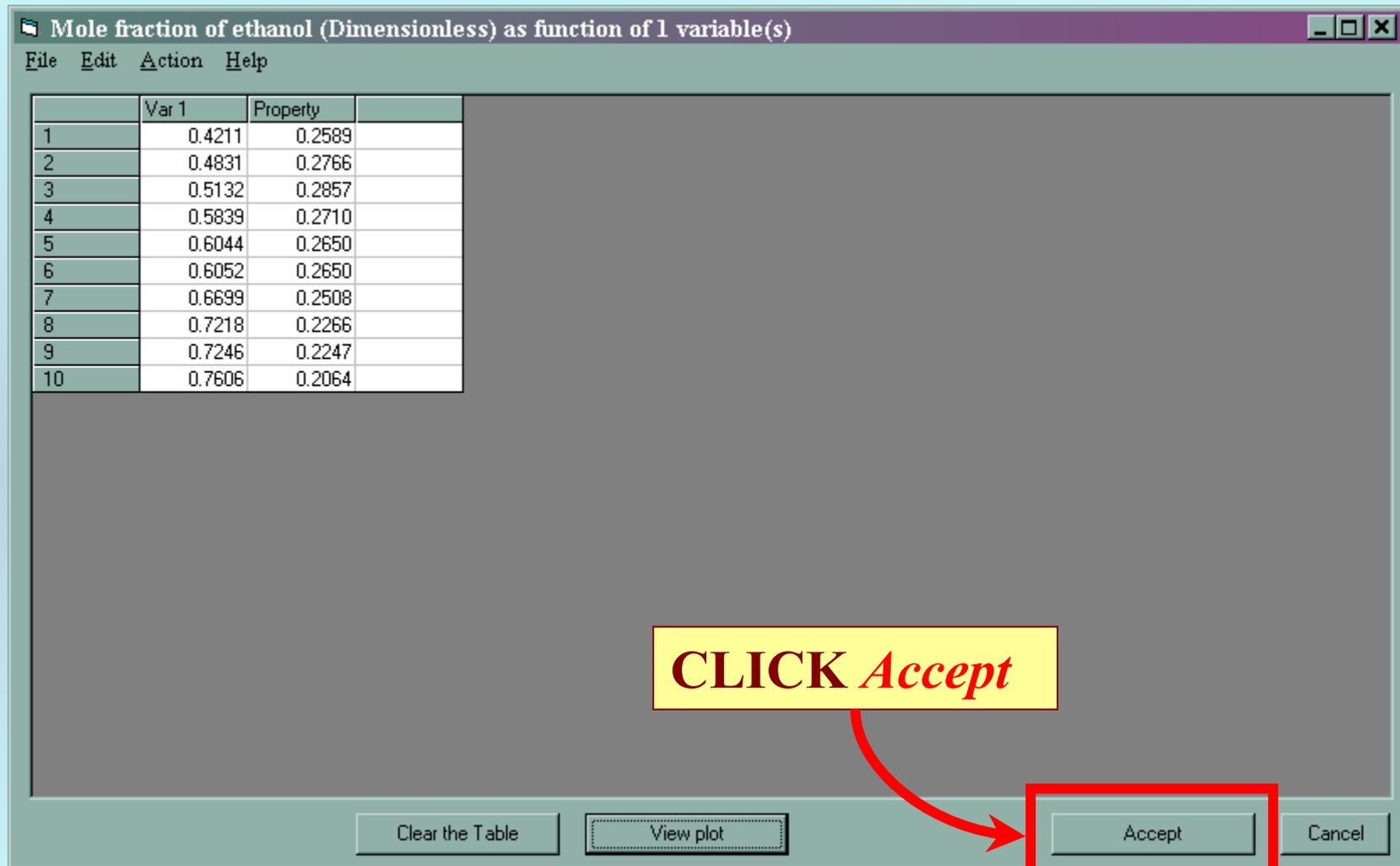
Mole fraction of ethanol (Dimensionless) as function of 1 variable(s)

File Edit Action Help

	Var 1	Property
1	0.4211	0.2589
2	0.4831	0.2766
3	0.5132	0.2857
4	0.5839	0.2710
5	0.6044	0.2650
6	0.6052	0.2650
7	0.6699	0.2508
8	0.7218	0.2266
9	0.7246	0.2247
10	0.7606	0.2064

**CLICK *Accept***

Clear the Table View plot **Accept** Cancel

The image shows a software window titled "Mole fraction of ethanol (Dimensionless) as function of 1 variable(s)". The window has a menu bar with "File", "Edit", "Action", and "Help". Below the menu bar is a table with three columns: an empty column, "Var 1", and "Property". The table contains 10 rows of data. At the bottom of the window, there are four buttons: "Clear the Table", "View plot", "Accept", and "Cancel". The "Accept" button is highlighted with a red rectangular box. A yellow callout box with a red border contains the text "CLICK *Accept*" in red, with a red arrow pointing from the callout box to the "Accept" button.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

- 2002 ben reh 0
  - dimethyl phthalate
    - Sample 1 (cm,99.0m%,nc;:)
  - diethyl phthalate
    - Sample 1 (cm,99.0m%,nc;se;)
  - dibutyl phthalate
    - Sample 1 (cm,99.0m%,nc;se;)
  - water
    - Sample 1 (cm;(Deionized with Milli-Q RG system);99.9m%,est)
  - ethanol
    - Sample 1 (cm,99.9m%,nc;:)
  - ethanol + dimethyl phthalate + water**
    - ^1: Ile, X1 (L1, Set 1), B Method:TITR**

**NOTE:** The new data set now appears in the 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.***