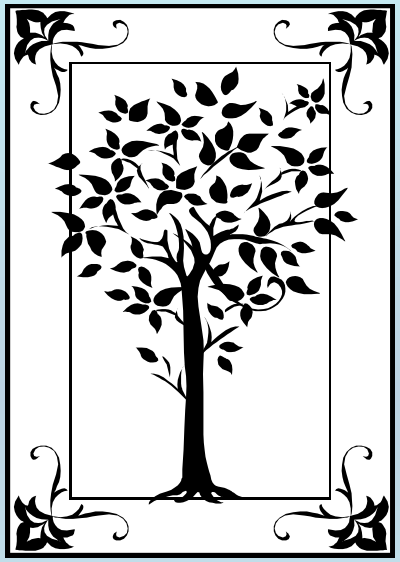
METADATA AND NUMERICAL DATA CAPTURE:
Liquid-Liquid Equilibrium - Binary
(Conjugate phase compositions – 2 Phases)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Liquid-Liquid Equilibrium (2 components)**
Conjugate Phase Compositions (2 Phases)
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:

J. Chem. Eng. Data 2003, *48*, 152−157

Liquid−Liquid Equilibrium and Excess Enthalpies in Binary Systems Methylcyclohexane + Methanol and Methylcyclohexane + *N*,*N*-Dimethylformamide

Magdalena Bendová,* Karel Řehák, Jaroslav Matouš, and Josef P. Novák

Department of Physical Chemistry, Institute of Chemical Technology, 166 28 Praha 6, Prague, Czech Republic

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Liquid−liquid equilibrium and excess enthalpies were studied for the two binary systems: methylcyclohexane + methanol and methylcyclohexane + *N*,*N*-dimethylformamide. Points of the binodal curve in the vicinity of the critical point were established in both of the systems by means of the cloud-point method. Equilibrium compositions were determined at different temperatures using the direct analytical method and the volume method. Excess enthalpies as functions of composition were determined at 298.15 K and 313.15 K using a Hart 4410 microcalorimeter with continuous-flow mixing cells. The results were correlated by the modified Wilson equation. A prediction of the liquid−liquid equilibrium and the excess enthalpy by the modified UNIFAC contribution method (Dortmund) was compared to the experimental values.

Conjugate phase compositions for (methylcyclohexane + methanol) at p = 101.3 kPa

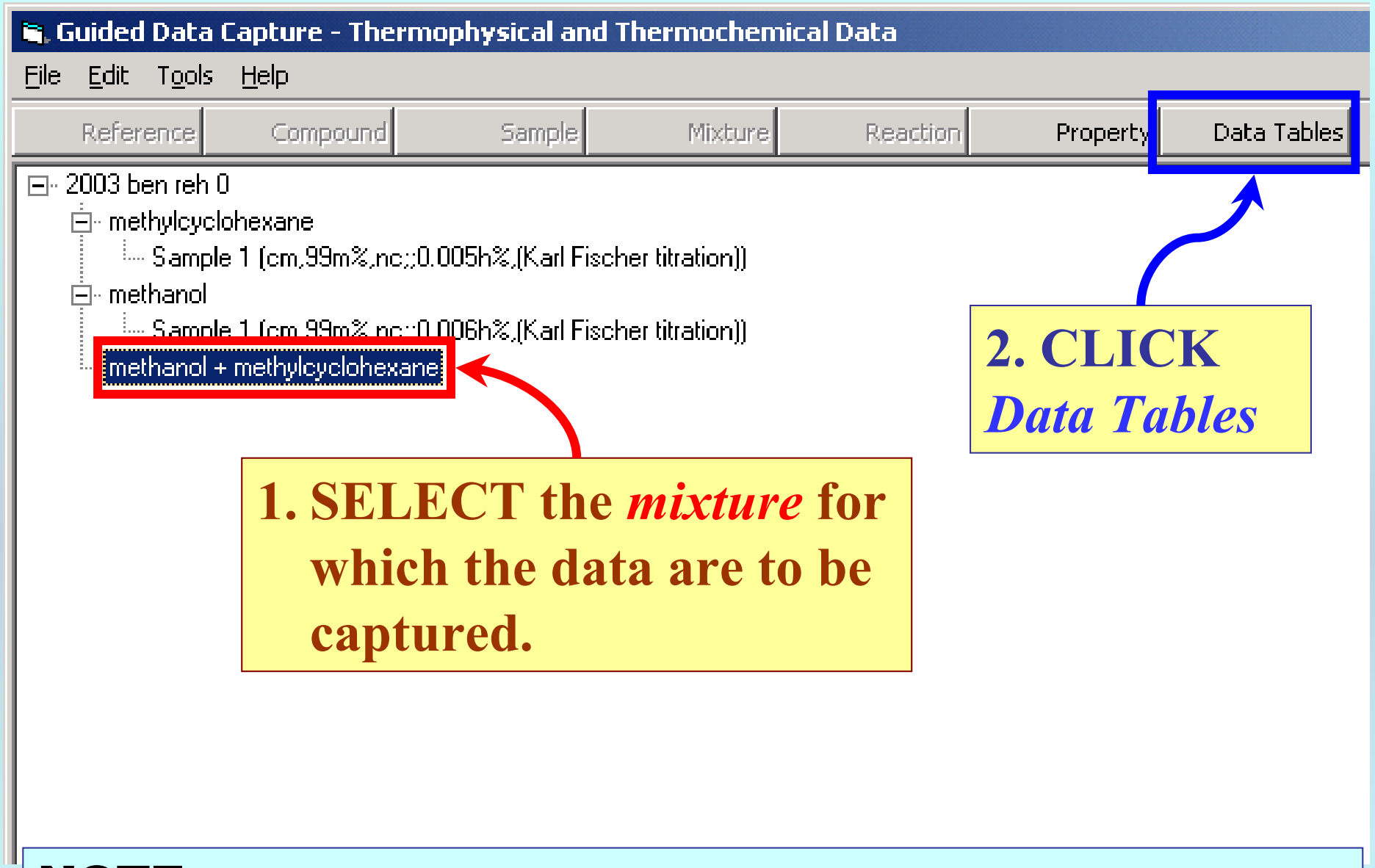
Table 3. Conjugated Phases Mole Fractions for the Systems Methylcyclohexane (1) + Methanol (2) and Methylcyclohexane (1) + *N*,*N*-DMF(2)

	solvent phase	alkane phase
T/K	x_1'	x_1''
Direct Analytical Method		
Methylcyclohexane (1) + Methanol (2)		
293.15	0.135	0.831
298.15	0.150	0.812
303.15	0.174	0.792
308.15	0.202	0.750
313.15	0.251	0.680

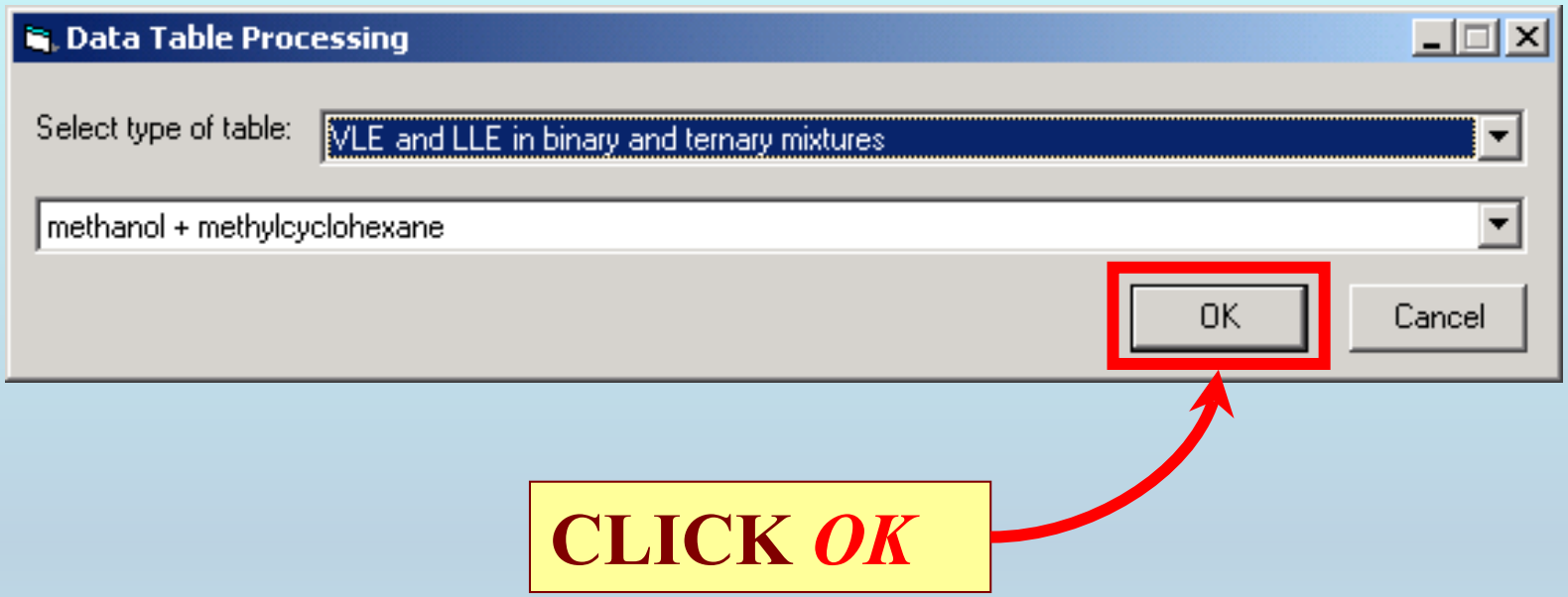
This data set is considered here.

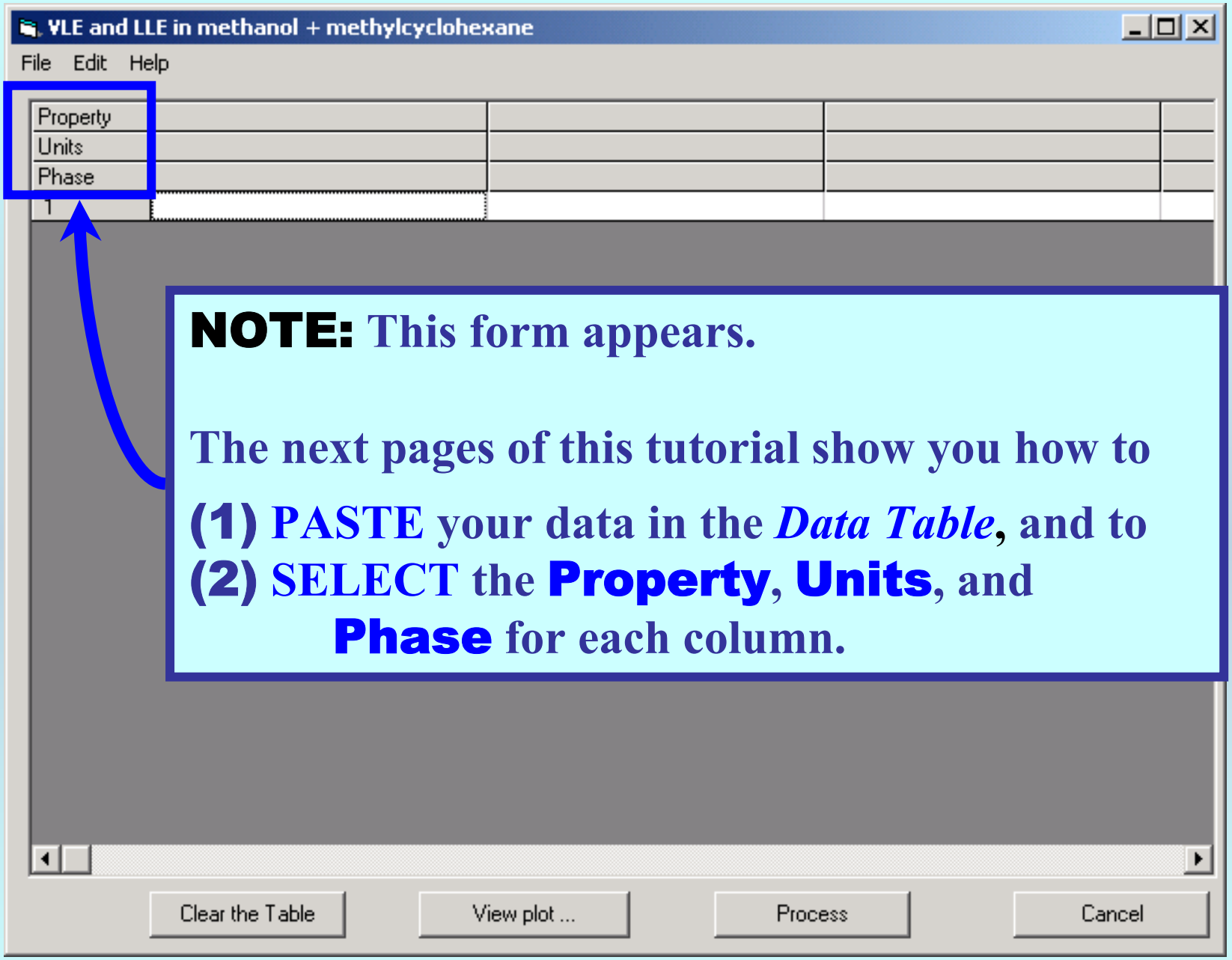
Experimental Method Info:

The direct analytical method consists of analyzing samples of the conjugated phases. In this work, capillary gas chromatography was employed. In the system methylcyclohexane + methanol, the concentration of methylcyclohexane was determined in both phases, because methanol was used as the GC solvent.



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.)


Data Table Processing
Select type of table:
VLE and LLE in binary and ternary mixtures
methanol + methylcyclohexane
OK
Cancel
CLICK *OK*


VLE and LLE in methanol + methylcyclohexane
File
Edit
Help
Property
Units
Phase
1
NOTE: This form appears.
The next pages of this tutorial show you how to
(1) PASTE your data in the Data Table, and to
(2) SELECT the Property, Units, and
Phase for each column.
Clear the Table
View plot ...
Process
Cancel

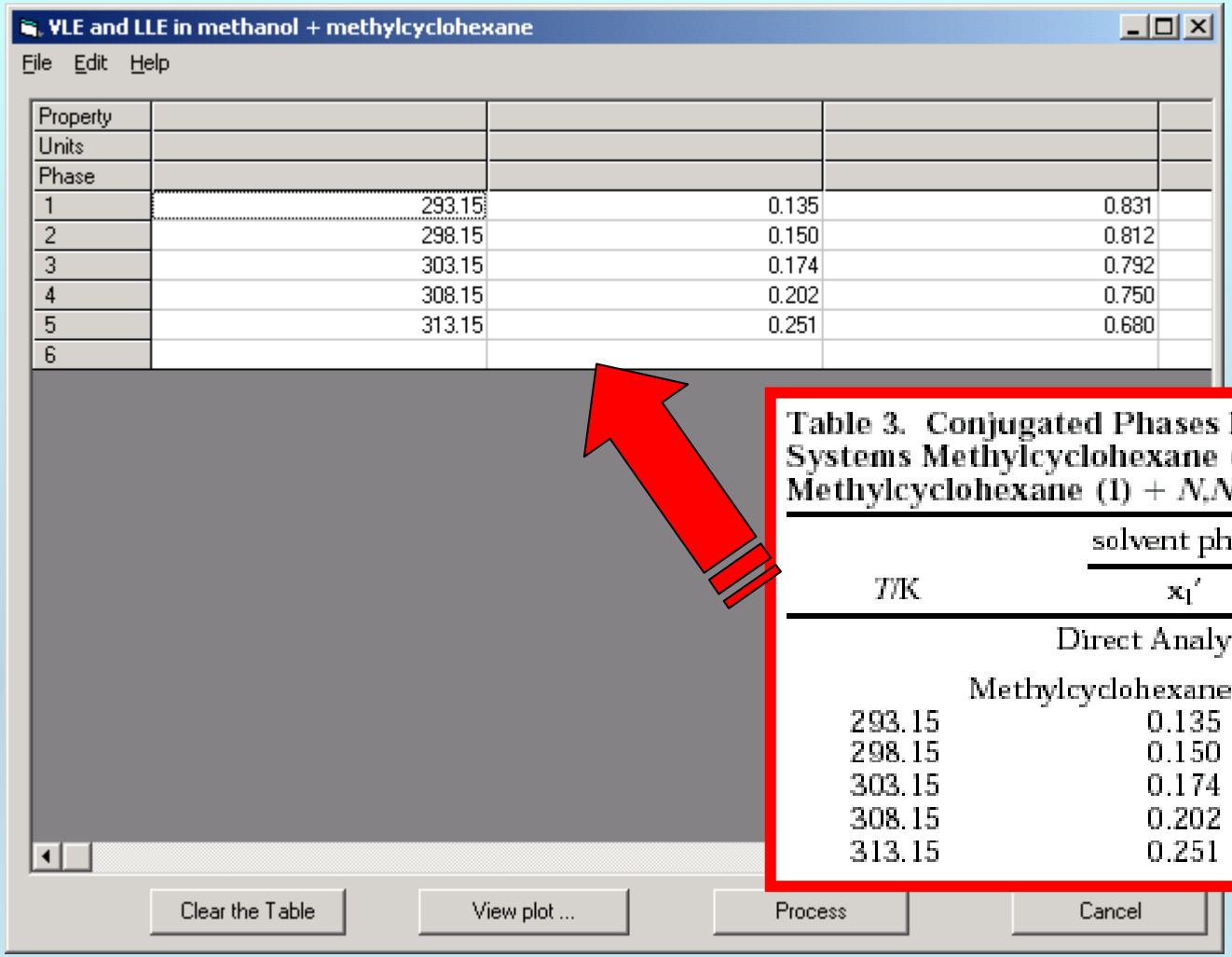


Table 3. Conjugated Phases Mole Fractions for the Systems Methylcyclohexane (1) + Methanol (2) and Methylcyclohexane (1) + *N,N*-DMF(2)

	solvent phase	alkane phase
T/K	x_1'	x_1''
Direct Analytical Method		
Methylcyclohexane (1) + Methanol (2)		
293.15	0.135	0.831
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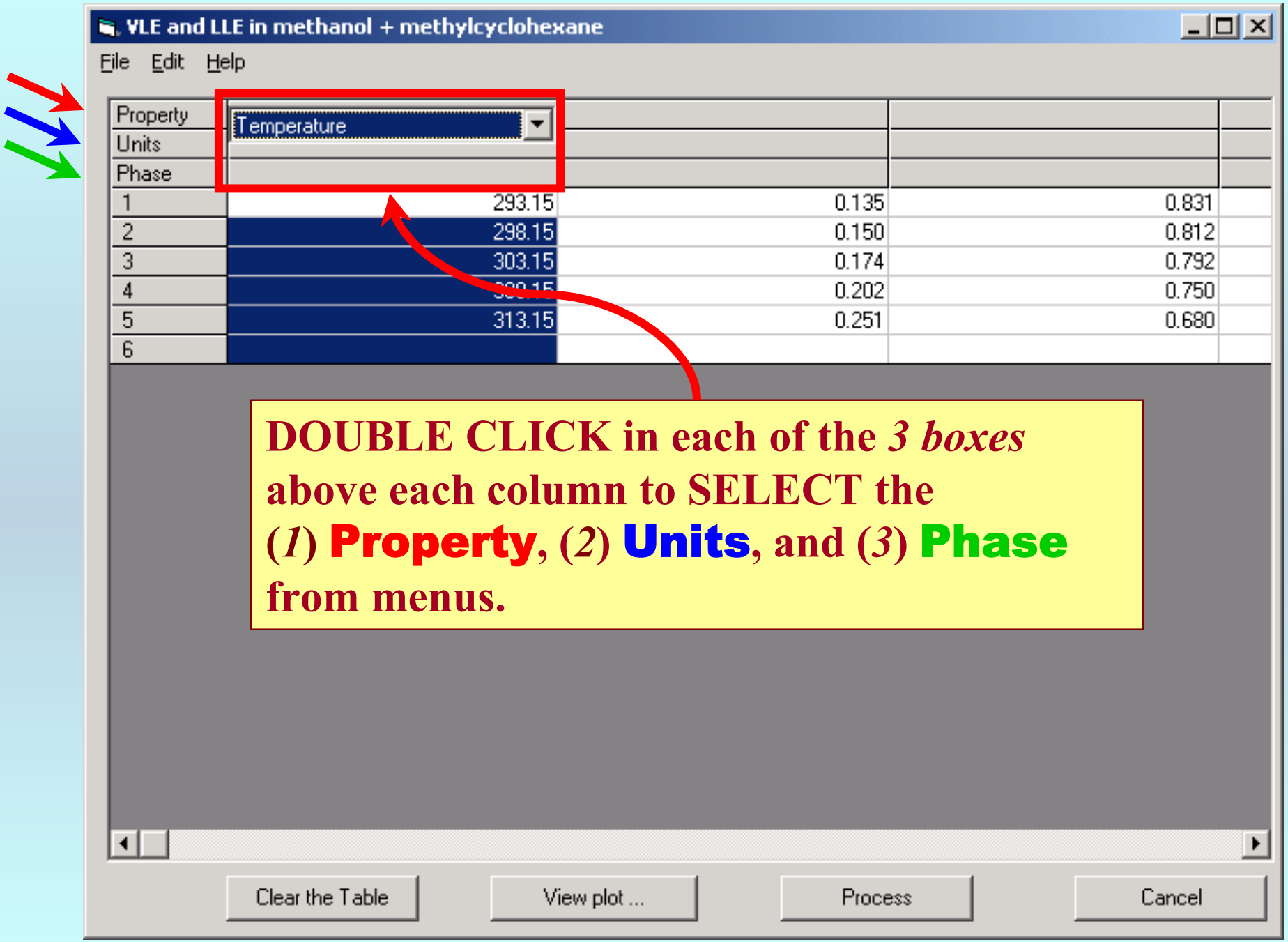
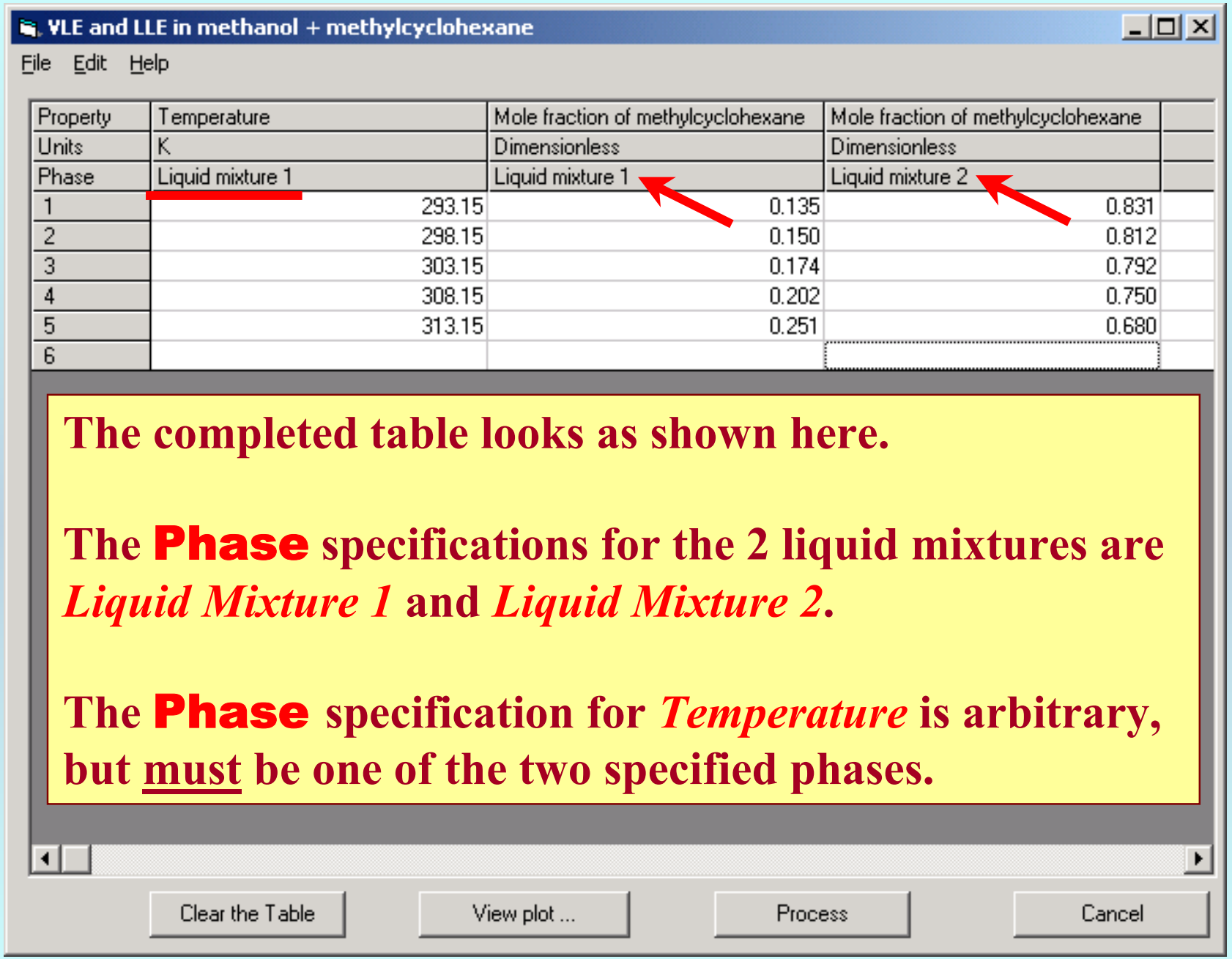
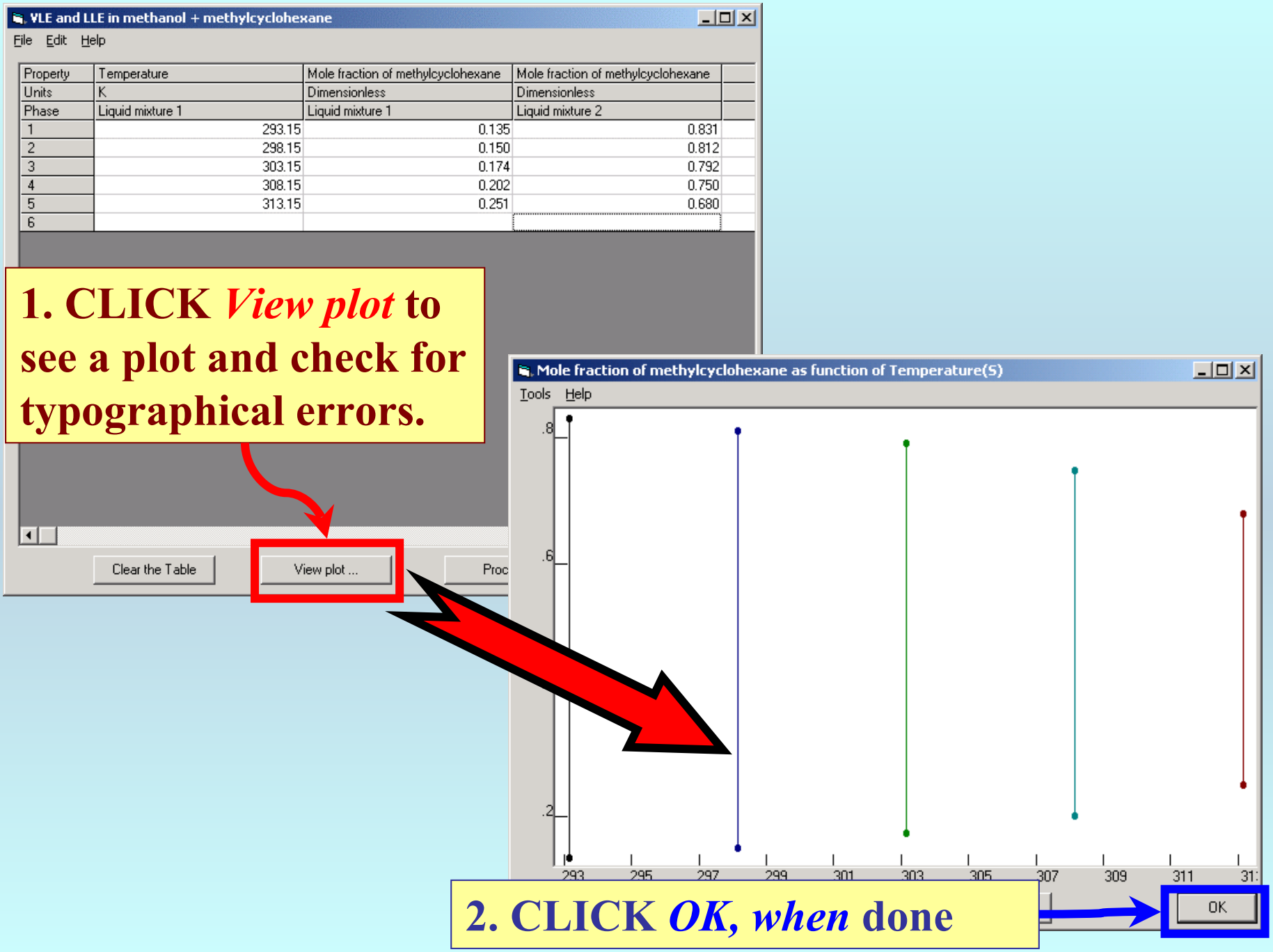
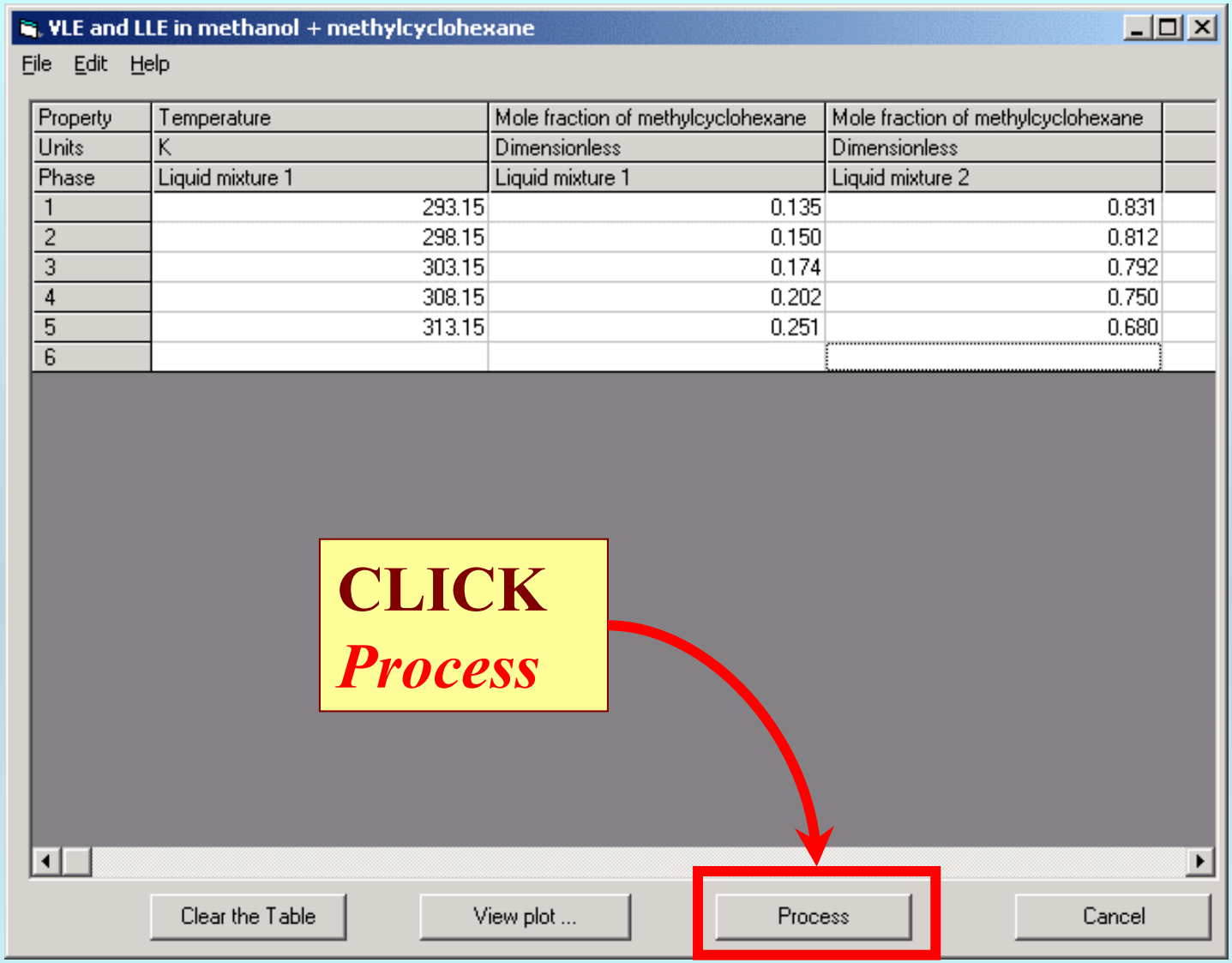
308.15	0.202	0.750
313.15	0.251	0.680

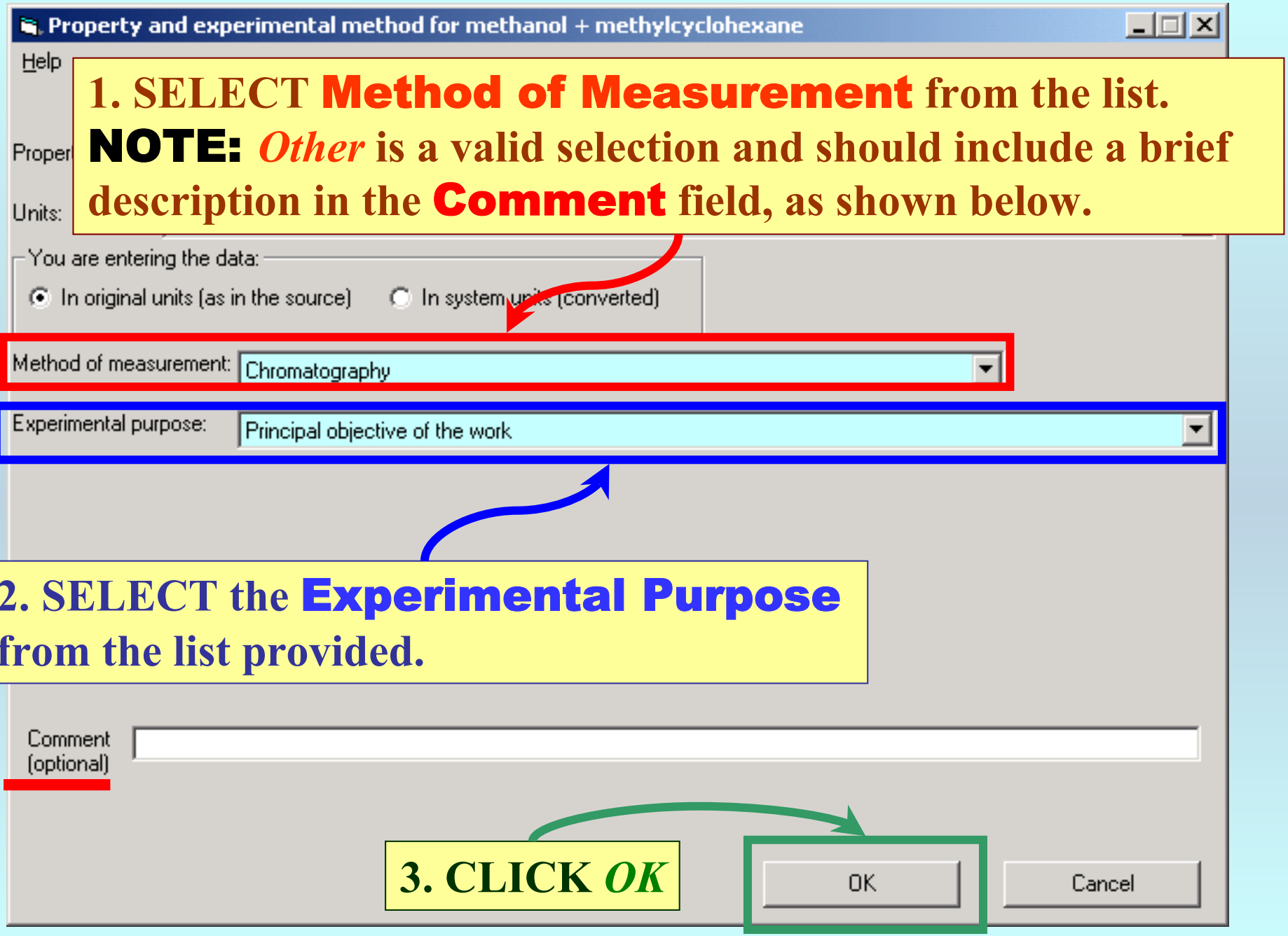
NOTE: Simple CUT/PASTE procedures can be used within the Data Table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

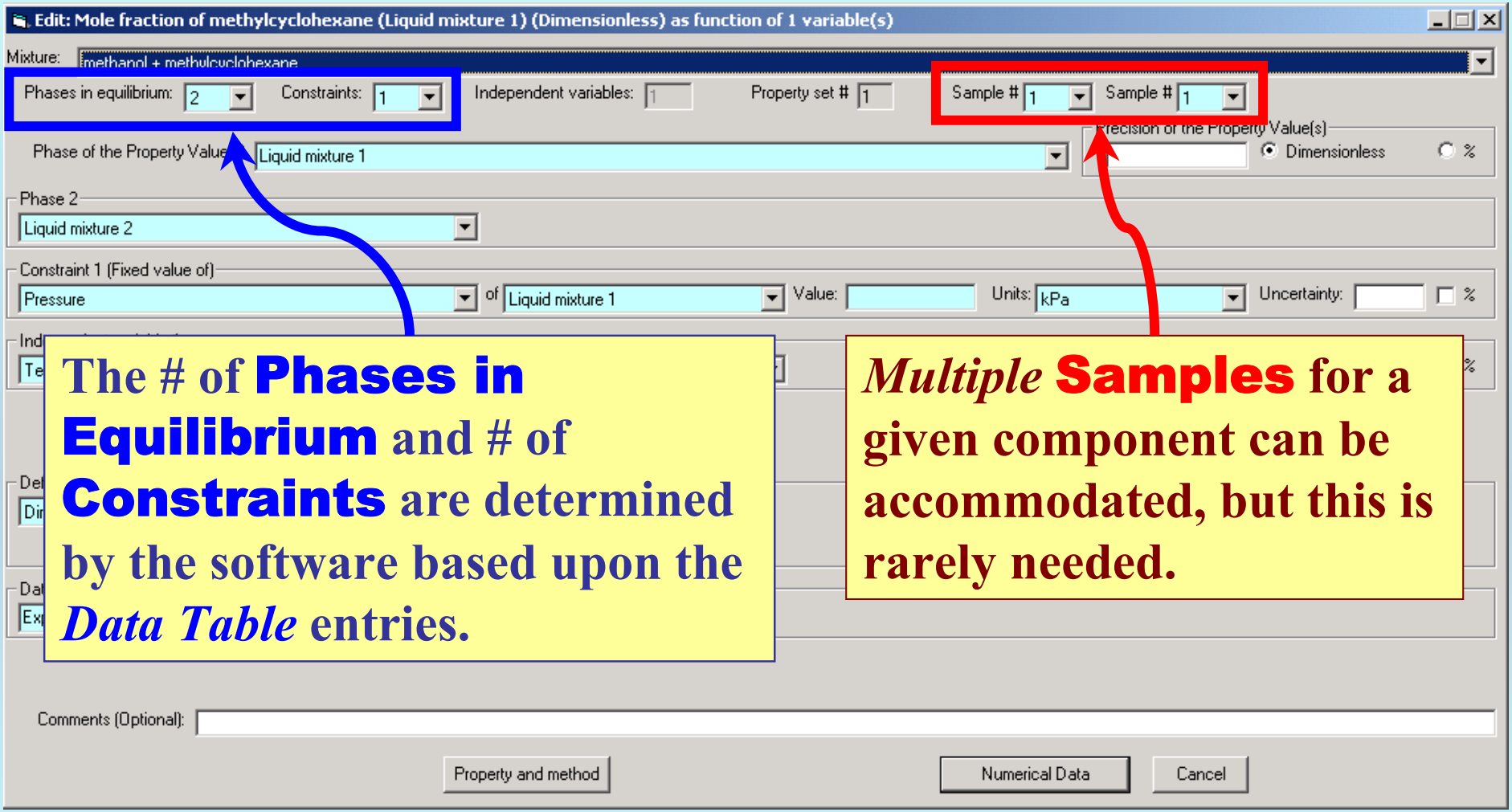

VLE and LLE in methanol + methylcyclohexane
File Edit Help
Property
Units
Phase
Temperature
1 293.15 0.135 0.831
2 298.15 0.150 0.812
3 303.15 0.174 0.792
4 0.202 0.750
5 313.15 0.251 0.680
6
DOUBLE CLICK in each of the 3 boxes above each column to SELECT the (1) Property, (2) Units, and (3) Phase from menus.
Clear the Table
View plot ...
Process
Cancel


VLE and LLE in methanol + methylcyclohexane
File Edit Help
Property | Temperature | Mole fraction of methylcyclohexane | Mole fraction of methylcyclohexane
Units | K | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2
1 | 293.15 | 0.135 | 0.831
2 | 298.15 | 0.150 | 0.812
3 | 303.15 | 0.174 | 0.792
4 | 308.15 | 0.202 | 0.750
5 | 313.15 | 0.251 | 0.680
6
The completed table looks as shown here.
The Phase specifications for the 2 liquid mixtures are Liquid Mixture 1 and Liquid Mixture 2.
The Phase specification for Temperature is arbitrary, but must be one of the two specified phases.
Clear the Table
View plot ...
Process
Cancel


VLE and LLE in methanol + methylcyclohexane
File Edit Help
Property | Temperature | Mole fraction of methylcyclohexane | Mole fraction of methylcyclohexane
Units | K | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2
1 | 293.15 | 0.135 | 0.831
2 | 298.15 | 0.150 | 0.812
3 | 303.15 | 0.174 | 0.792
4 | 308.15 | 0.202 | 0.750
5 | 313.15 | 0.251 | 0.680
6
1. CLICK View plot to see a plot and check for typographical errors.
Clear the Table
View plot ...
Proc
Mole fraction of methylcyclohexane as function of Temperature(S)
Tools Help
.8
.6
.2
293 295 297 299 301 303 305 307 309 311
2. CLICK OK, when done
OK


VLE and LLE in methanol + methylcyclohexane
File Edit Help
Property | Temperature | Mole fraction of methylcyclohexane | Mole fraction of methylcyclohexane
Units | K | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2
1 | 293.15 | 0.135 | 0.831
2 | 298.15 | 0.150 | 0.812
3 | 303.15 | 0.174 | 0.792
4 | 308.15 | 0.202 | 0.750
5 | 313.15 | 0.251 | 0.680
6
CLICK
Process
Clear the Table
View plot ...
Process
Cancel


Property and experimental method for methanol + methylcyclohexane
Help
Proper
Units:
1. SELECT Method of Measurement from the list.
NOTE: Other is a valid selection and should include a brief description in the Comment field, as shown below.
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Chromatography
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
3. CLICK OK
OK
Cancel

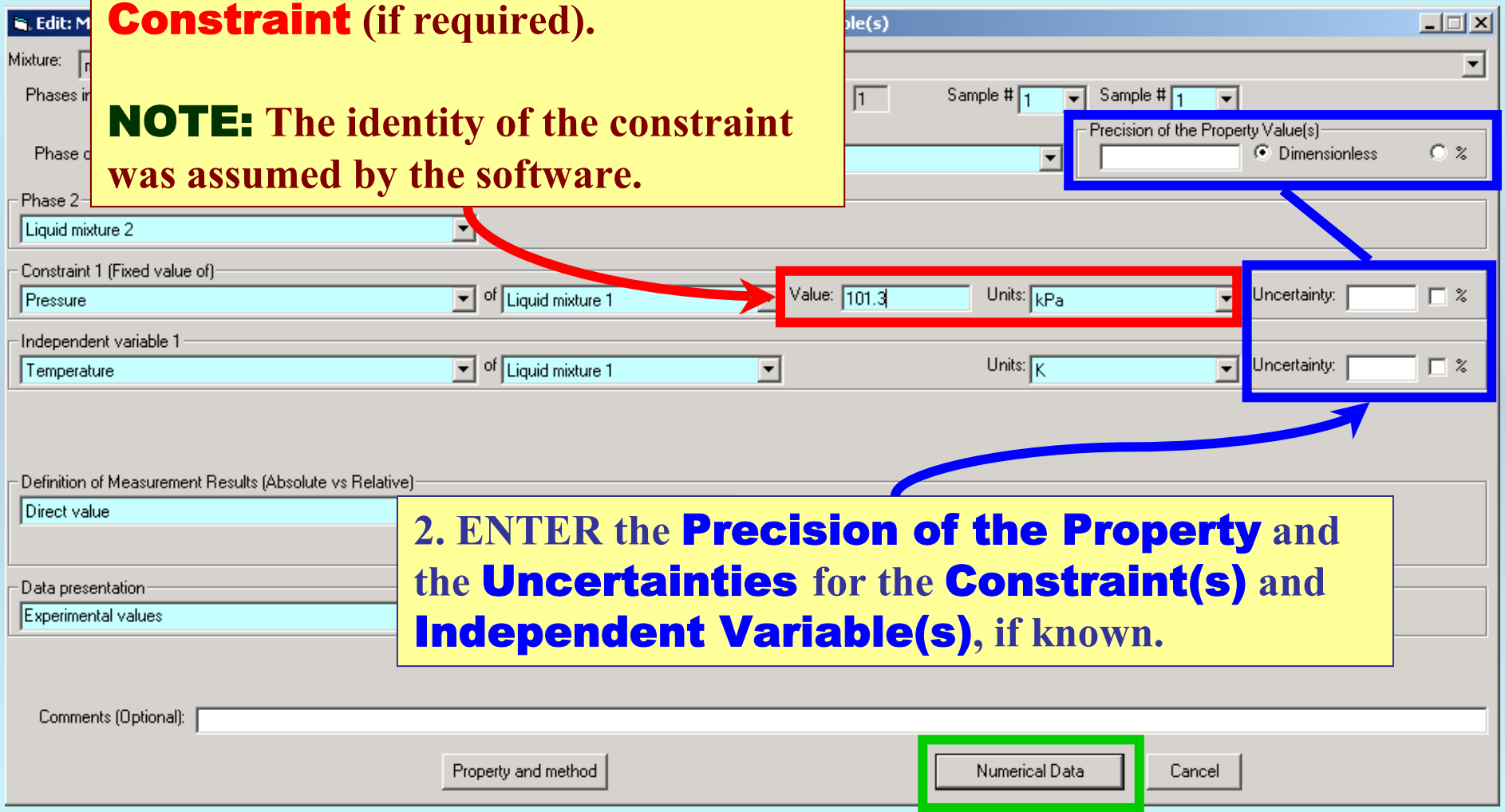


The # of **Phases in Equilibrium** and # of **Constraints** are determined by the software based upon the *Data Table* entries.

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

1. TYPE the **Value** (*101.3*, here) and SELECT the **Units** (*kPa*, here) for the **Constraint** (if required).

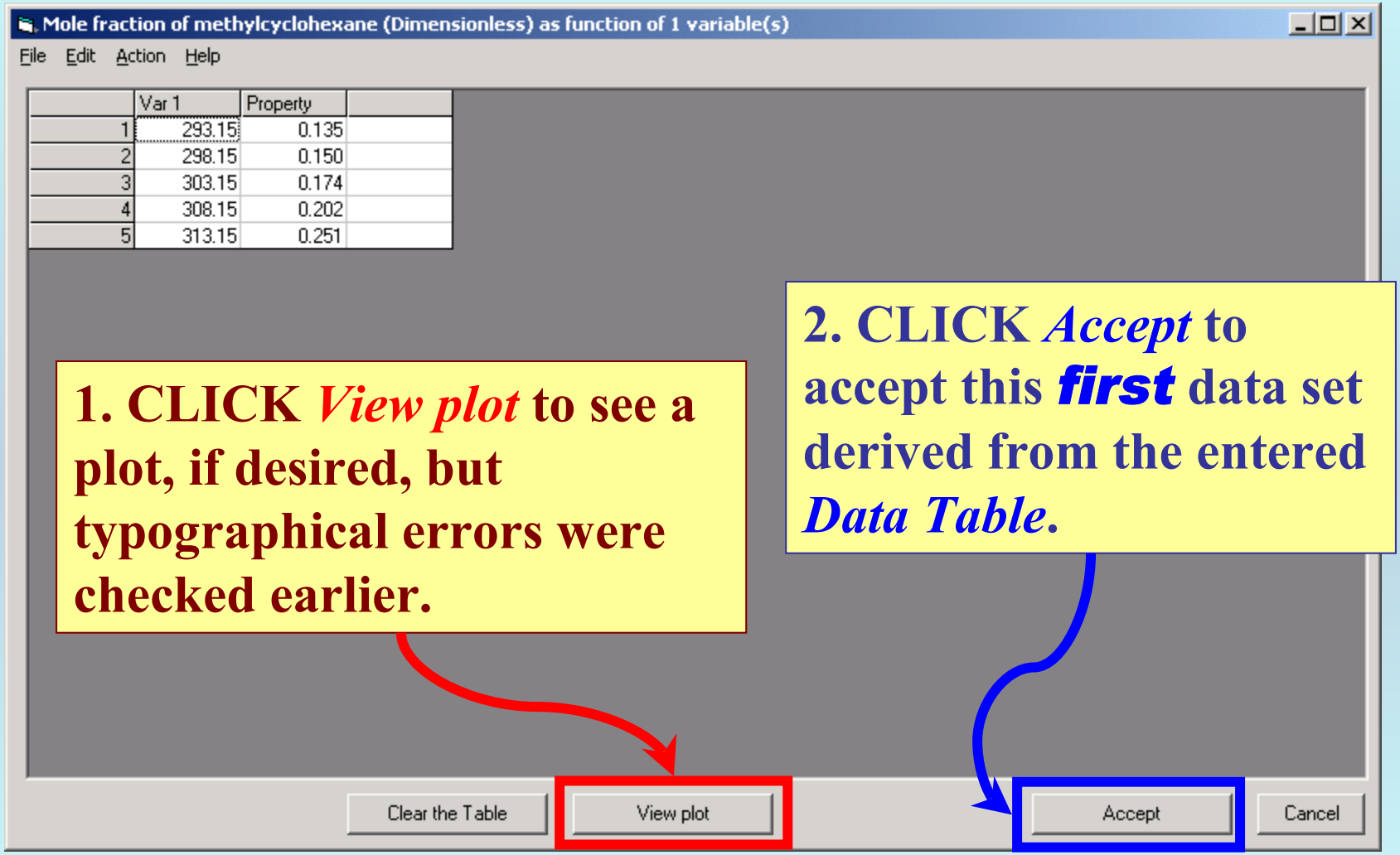
NOTE: The identity of the constraint was assumed by the software.

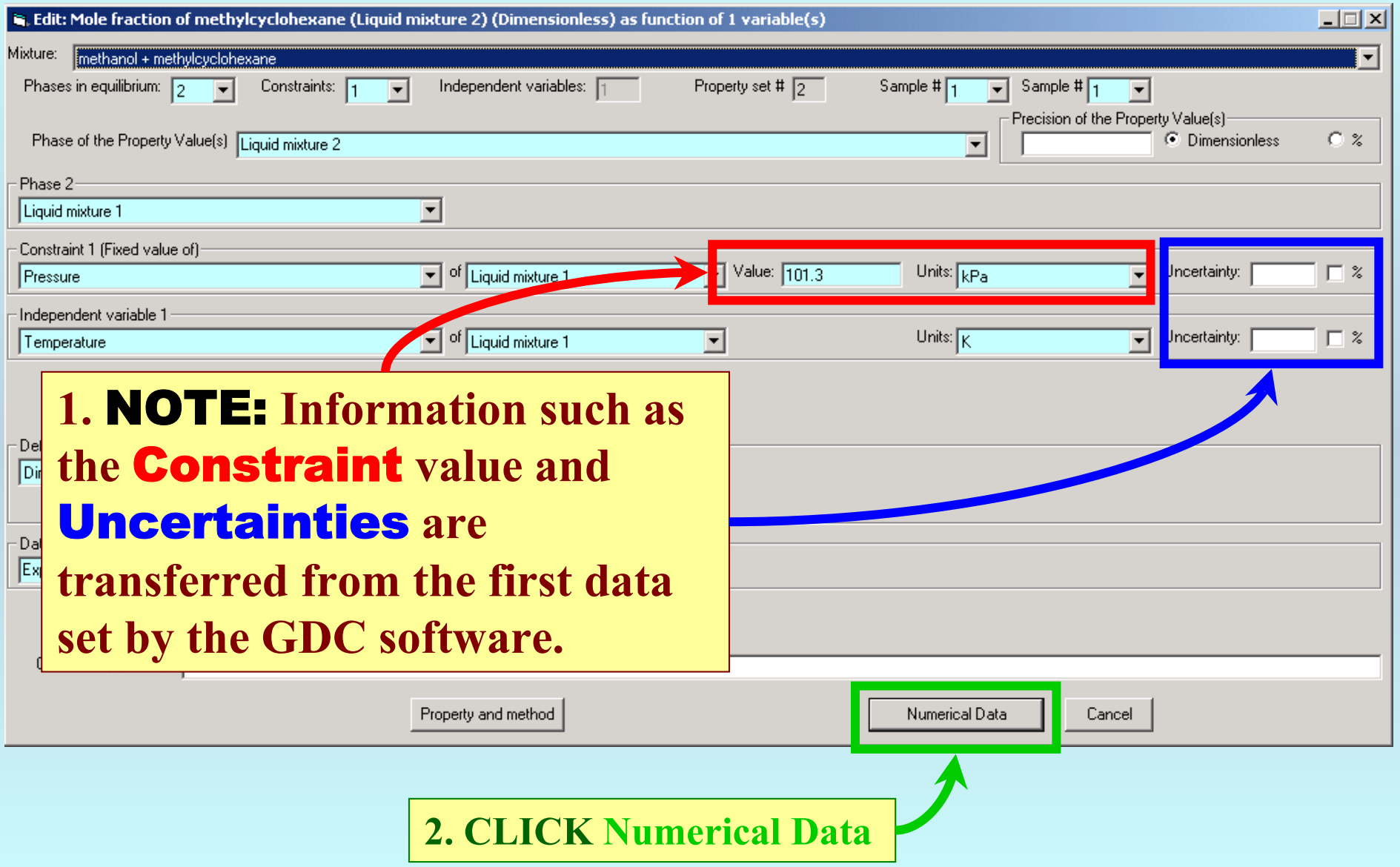


2. ENTER the **Precision of the Property** and the **Uncertainties** for the **Constraint(s)** and **Independent Variable(s)**, if known.

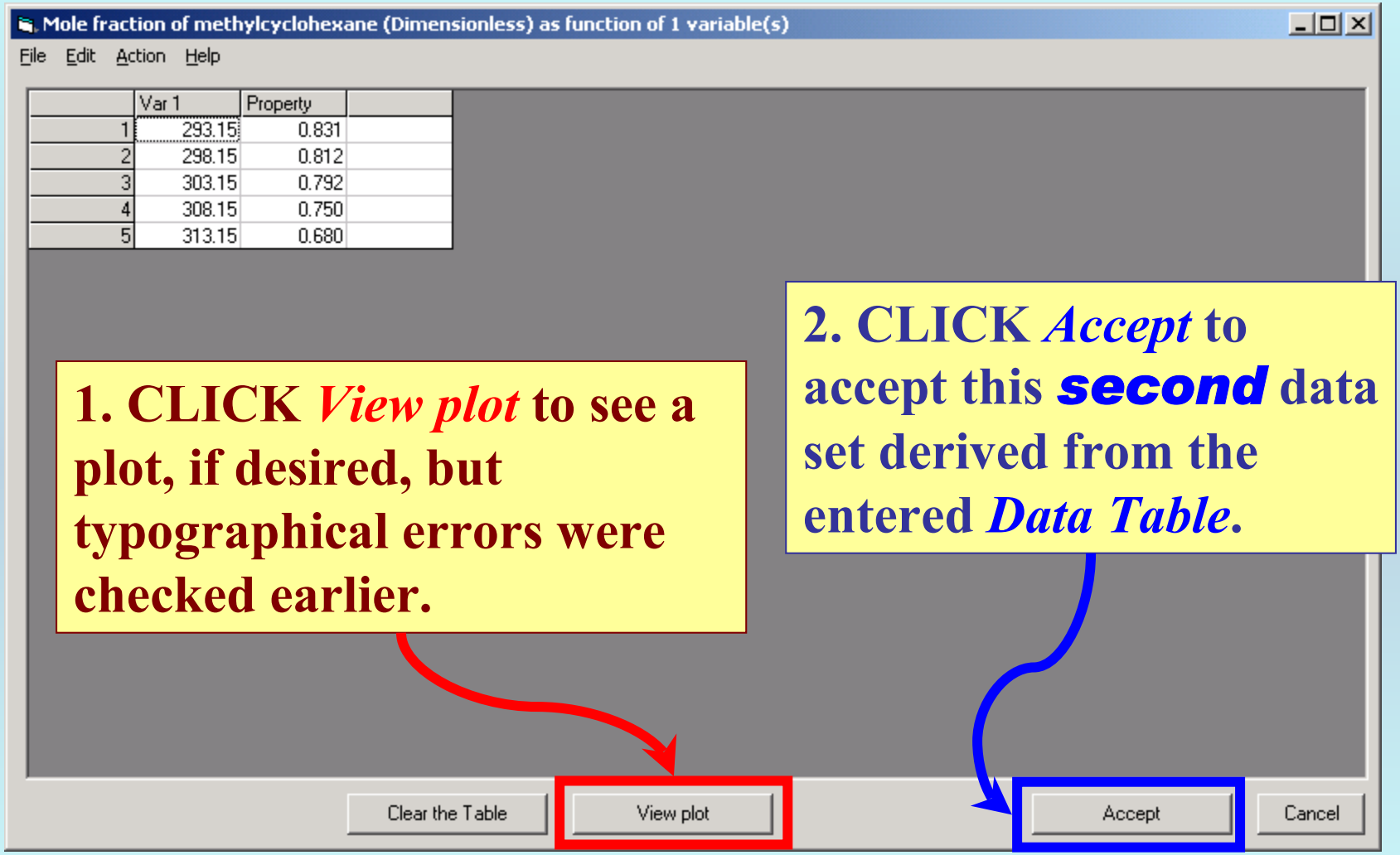
3. CLICK Numerical Data

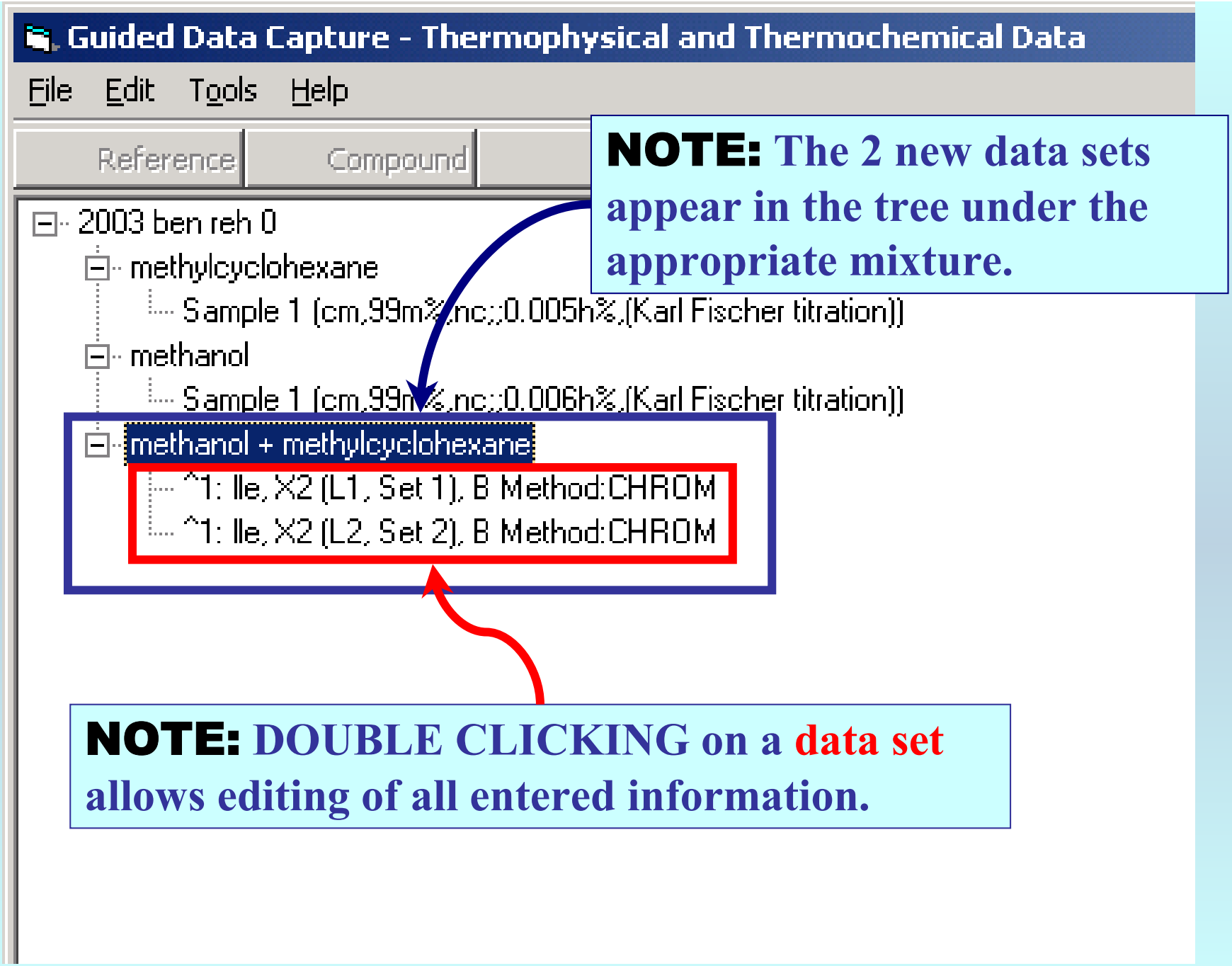
Note: The numerical data shown here were transferred by the software from the ***Data Table*** entered previously.




Edit: Mole fraction of methylcyclohexane (Liquid mixture 2) (Dimensionless) as function of 1 variable(s)
Mixture: methanol + methylcyclohexane
Phases in equilibrium: 2
Constraints: 1
Independent variables: 1
Property set # 2
Sample # 1
Sample # 1
Phase of the Property Value(s): Liquid mixture 2
Precision of the Property Value(s)
Dimensionless
%
Phase 2
Liquid mixture 1
Constraint 1 (Fixed value of)
Pressure
of Liquid mixture 1
Value: 101.3
Units: kPa
Uncertainty:
%
Independent variable 1
Temperature
of Liquid mixture 1
Units: K
Uncertainty:
%
1. NOTE: Information such as the Constraint value and Uncertainties are transferred from the first data set by the GDC software.
Property and method
Numerical Data
Cancel
2. CLICK Numerical Data

Note: The numerical data shown here were, ***also***, transferred by the software from the ***Data Table*** entered previously.




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
2003 ben reh 0
methylcyclohexane
Sample 1 (cm,99m%,nc;;0.005h%,(Karl Fischer titration))
methanol
Sample 1 (cm,99m%,nc;;0.006h%,(Karl Fischer titration))
methanol + methylcyclohexane
^1: Ile, X2 (L1, Set 1), B Method:CHROM
^1: Ile, X2 (L2, Set 2), B Method:CHROM
NOTE: The 2 new data sets appear in the tree under the appropriate mixture.
NOTE: DOUBLE CLICKING on a 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.**