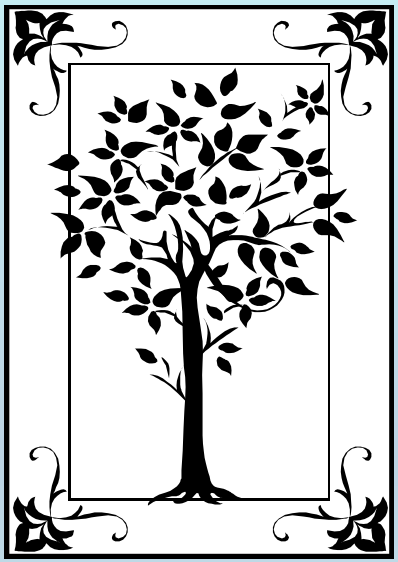
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY
(1 component in supercritical CO_2)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY
(1 component in supercritical CO_2)
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 2001, *46*, 647−650

Solubilities of Azobenzene, *p*-Hydroxyazobenzene, and *p*-Dimethylaminoazobenzene in Supercritical Carbon Dioxide

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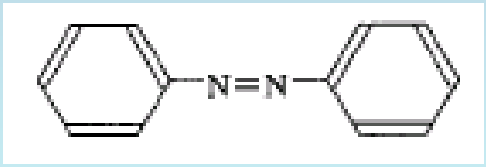
The solubilities of azobenzene, *p*-hydroxyazobenzene, and *p*-dimethylaminoazobenzene which were suitable for dyeing from supercritical carbon dioxide (SC-CO_2) were measured at 308.2 K and 318.2 K over the pressure range from 9.1 MPa to 25.3 MPa by a flow type apparatus. The solubilities were determined from the mass of solute trapped by decompression and the volume of released CO_2. Solubility data were correlated by a solution model based on the regular solution concept.

SOLUBILITY of 1 component in supercritical CO_2
Azobenzene + CO_2

Table 1. Mole Fraction Solubilities, y_2, of Azobenzene, *p*-Hydroxyazobenzene, and *p*-Dimethylaminoazobenzene in SC-CO_2

azobenzene				*p*-hydroxyazobenzene				*p*-dimethylaminoazobenzene			
$T = 308.2$ K		$T = 318.2$ K		$T = 308.2$ K		$T = 318.2$ K		$T = 308.2$ K		$T = 318.2$ K	
p/MPa	$10^3 y_2$	p/MPa	$10^3 y_2$	p/MPa	$10^3 y_2$	p/MPa	$10^3 y_2$	p/MPa	$10^4 y_2$	p/MPa	$10^4 y_2$
9.1	3.64	9.1	2.99	9.1	2.57	9.1	1.83	9.1	4.37	9.1	3.22
10.1	4.06	10.1	5.13	10.1	2.75	10.1	3.29	10.1	4.67	10.1	5.37
15.2	5.04	15.2	8.24	15.2	3.45	15.2	5.16	15.2	7.24	15.2	10.3
20.3	5.54	20.3	9.26	20.3	3.54	20.3	5.93	20.3	8.29	20.3	12.3
25.3	5.98	25.3	9.84	25.3	3.95	25.3	6.36	25.3	9.05	24.5	12.5

This data set is considered here.

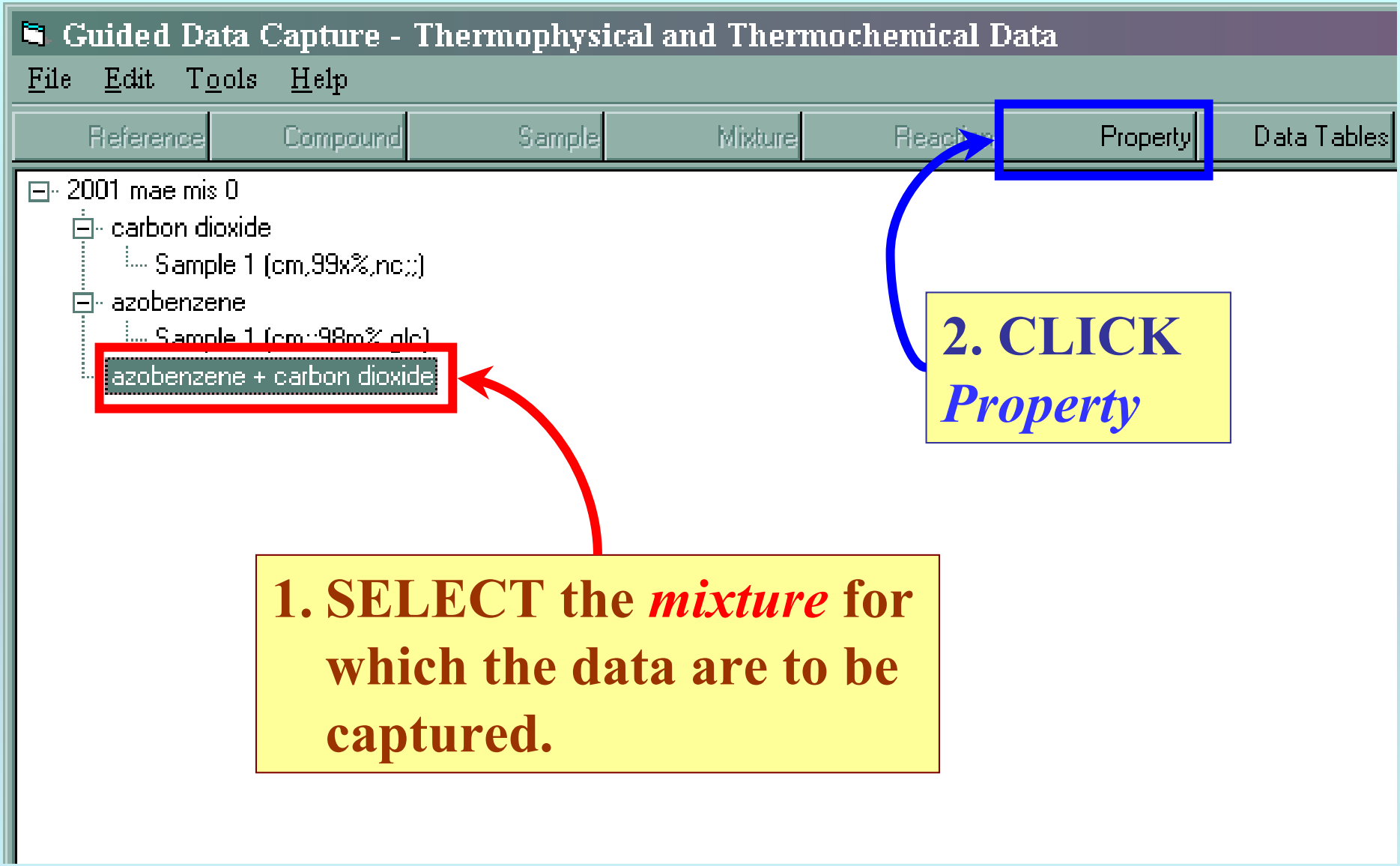


Experimental Method & Uncertainty Estimates:

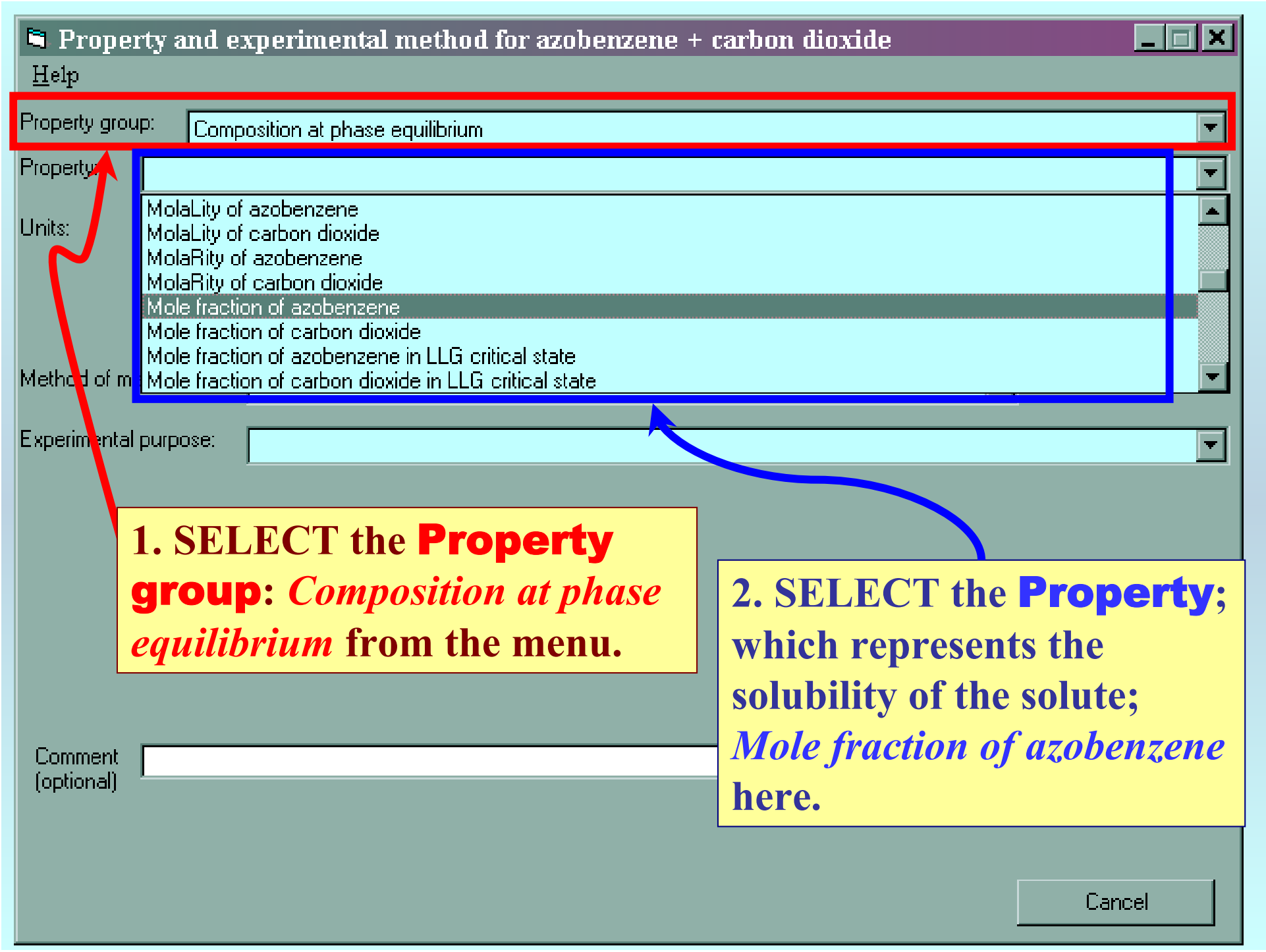
These cells were attached to a preheating coil and submerged in a water bath controlled with a temperature control accuracy of ±0.1 K. The supercritical fluid (SCF) saturated with the solid component was decompressed through an expansion valve and introduced into a U-shaped glass tube cooled in an ice bath. Gaseous CO_2 and the solid component were separated in the tube. The amount of the trapped solid component was determined by mass.

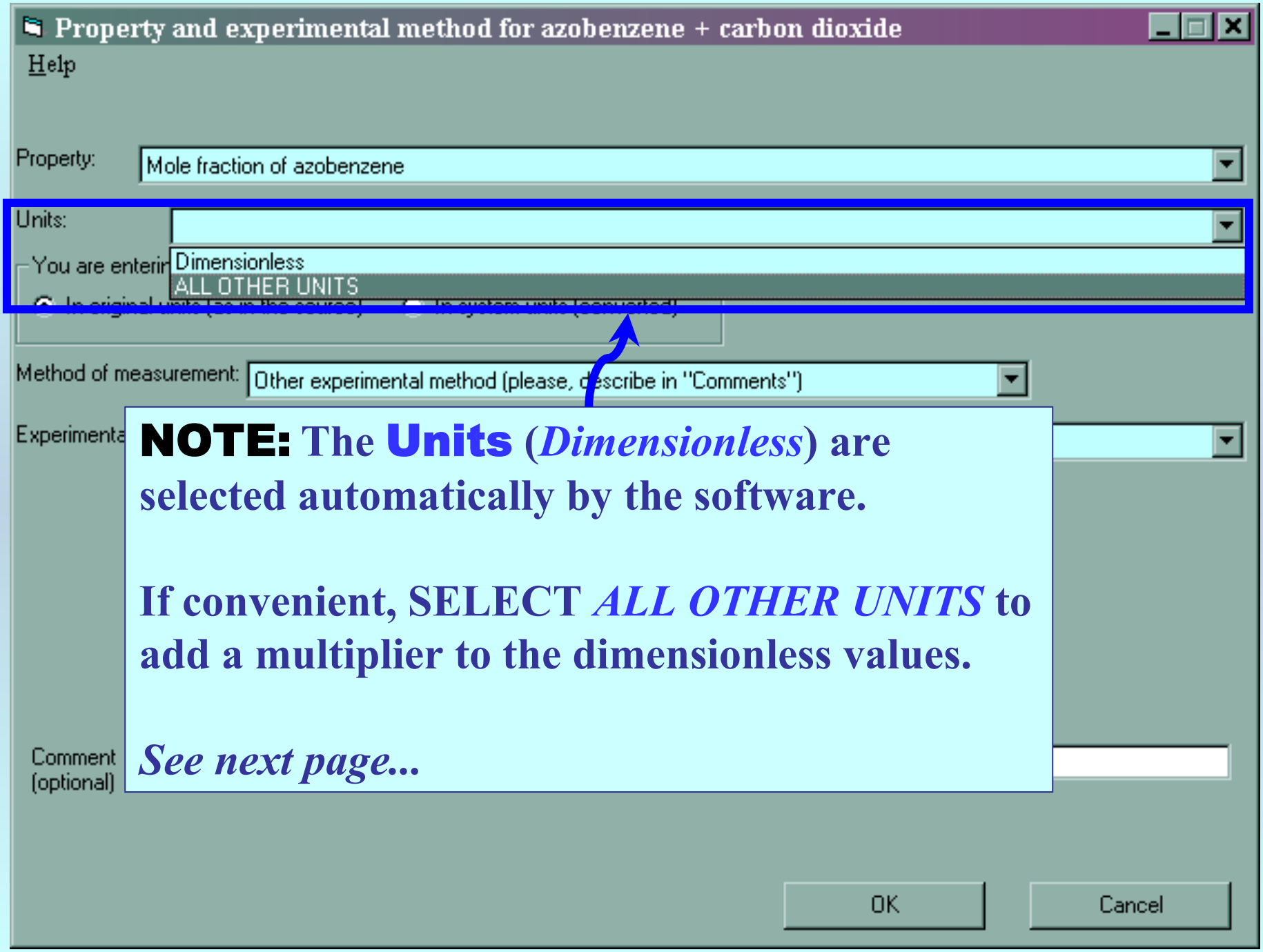
A back-pressure regulator was used to maintain a constant pressure with the pressure control accuracy of ±0.1 MPa.

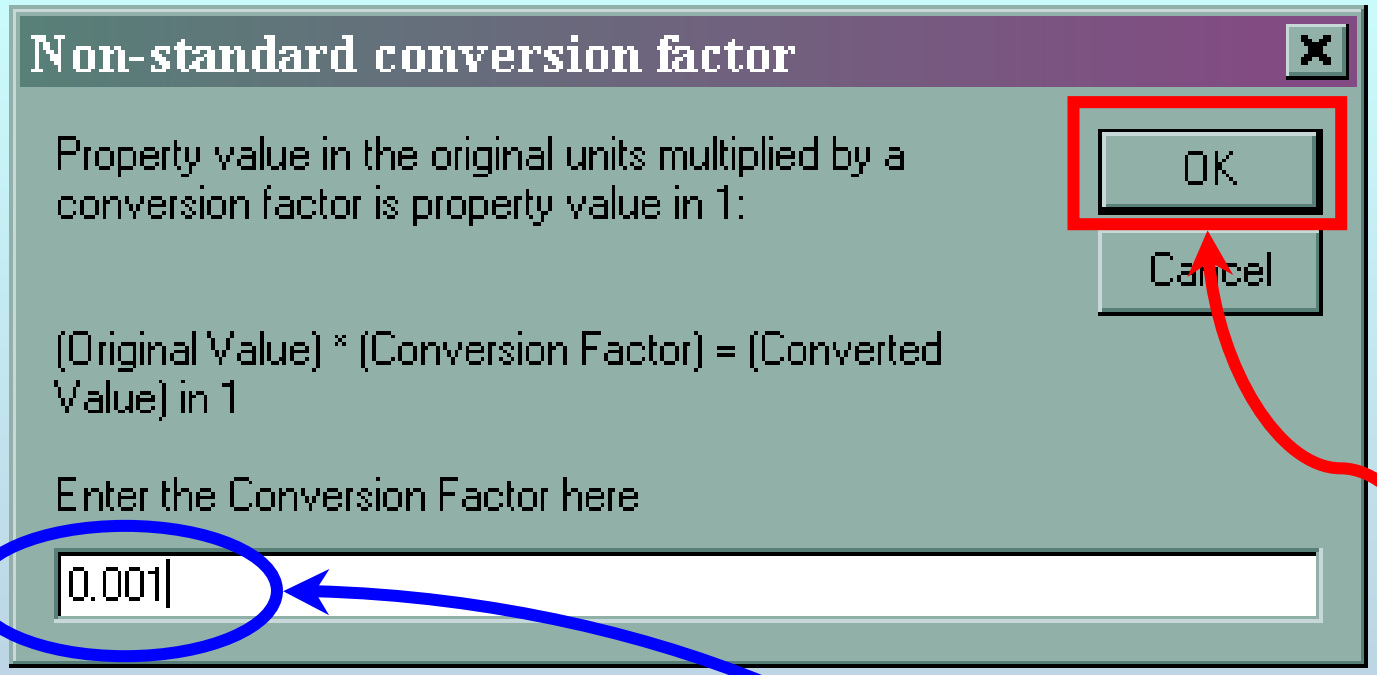
The reproducibility of these solubilities was within ±4.0%



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 azobenzene + carbon dioxide
Help
Property group:
Composition at phase equilibrium
Property:
Units:
MolaLity of azobenzene
MolaLity of carbon dioxide
MolaRity of azobenzene
MolaRity of carbon dioxide
Mole fraction of azobenzene
Mole fraction of carbon dioxide
Mole fraction of azobenzene in LLG critical state
Mole fraction of carbon dioxide in LLG critical state
Experimental purpose:
1. SELECT the Property group: Composition at phase equilibrium from the menu.
2. SELECT the Property; which represents the solubility of the solute; Mole fraction of azobenzene here.
Comment (optional)
Cancel

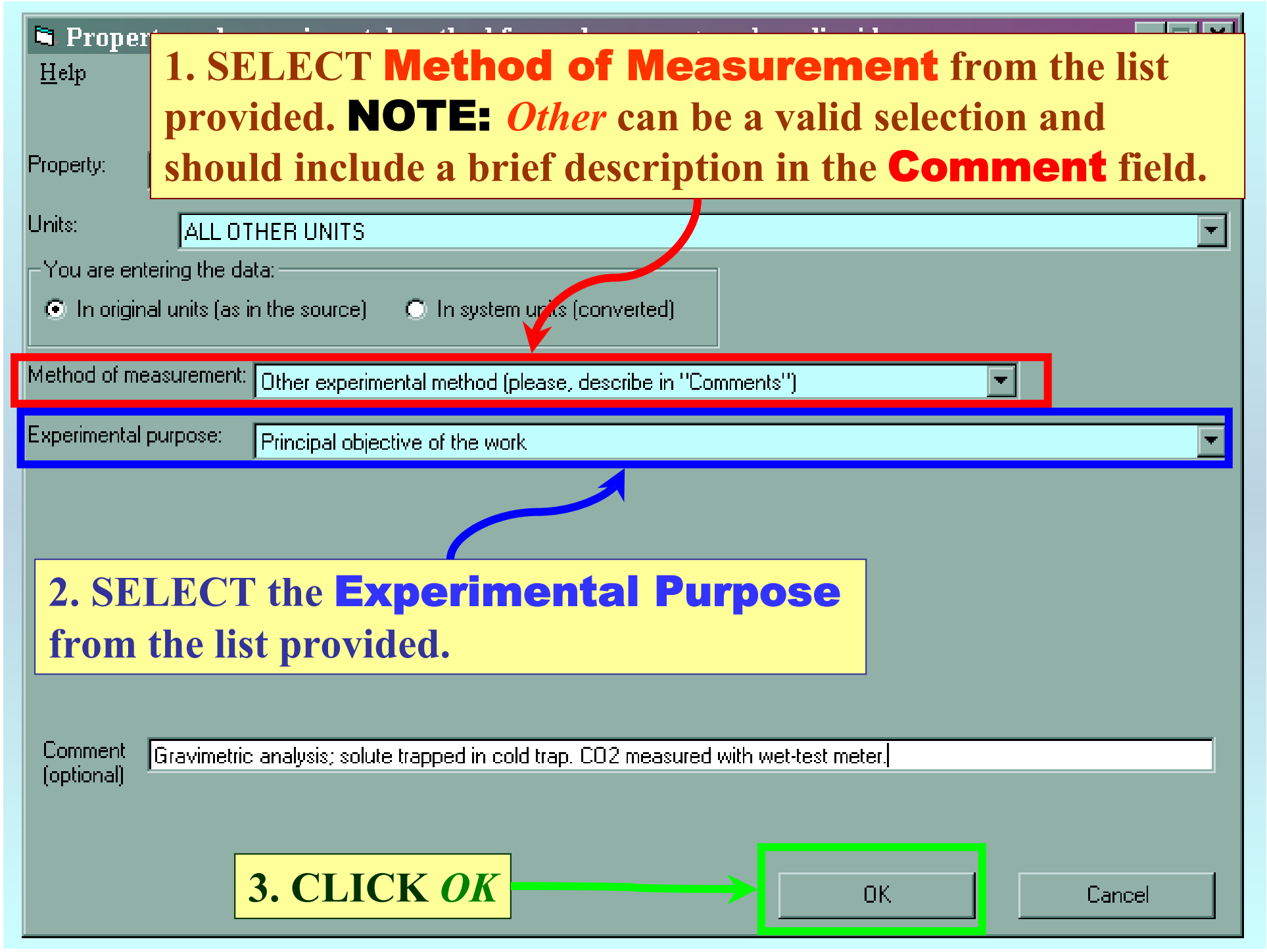

Property and experimental method for azobenzene + carbon dioxide
Help
Property:
Mole fraction of azobenzene
Units:
Dimensionless
ALL OTHER UNITS
You are enterir
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimenta
NOTE: The Units (Dimensionless) are selected automatically by the software.
If convenient, SELECT ALL OTHER UNITS to add a multiplier to the dimensionless values.
See next page...
Comment (optional)
OK
Cancel



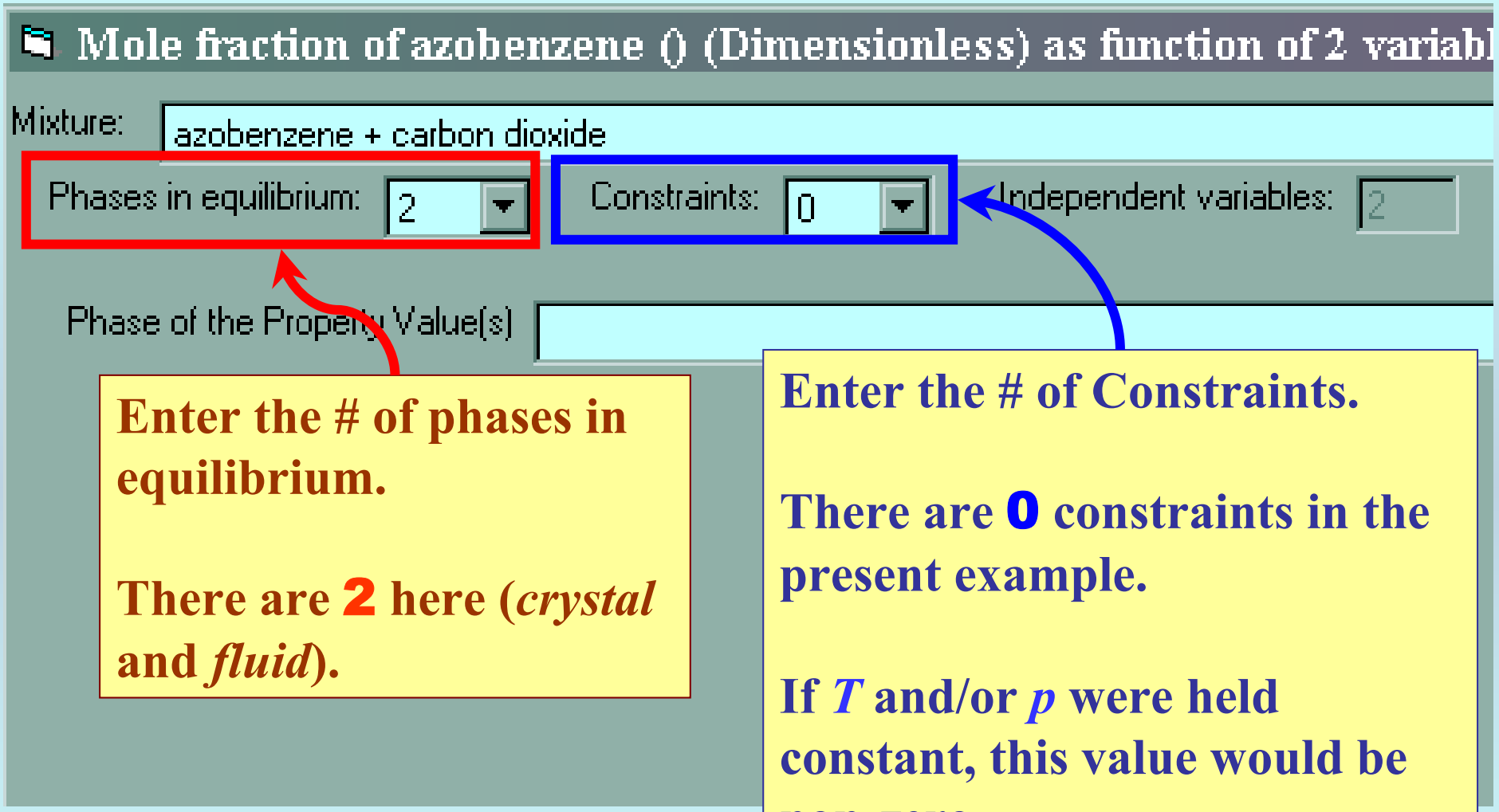
azobenzene

$T = 308.2$ K		$T = 318.2$ K	
p/MPa	$10^3 y_2$	p/MPa	$10^3 y_2$
9.1	3.64	9.1	2.99
10.1	4.06	10.1	5.13
15.2	5.04	15.2	8.24
20.3	5.54	20.3	9.26
25.3	5.98	25.3	9.84

CLICK *OK*, after entry of the *Conversion Factor*.


Help
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.
Property:
Units:
ALL OTHER UNITS
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
Gravimetric analysis; solute trapped in cold trap. CO2 measured with wet-test meter.
3. CLICK OK
OK
Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints



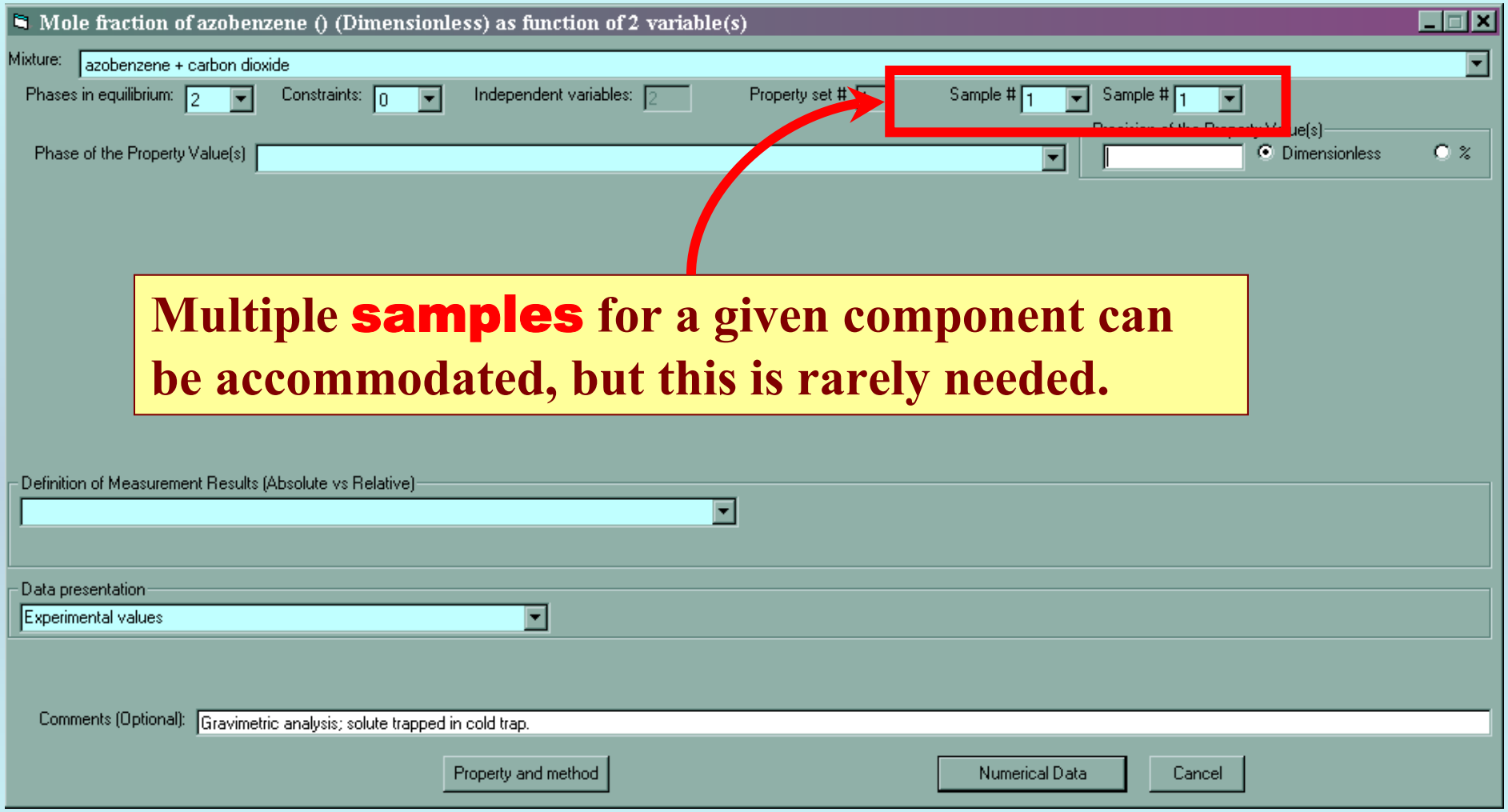
Enter the # of phases in equilibrium.

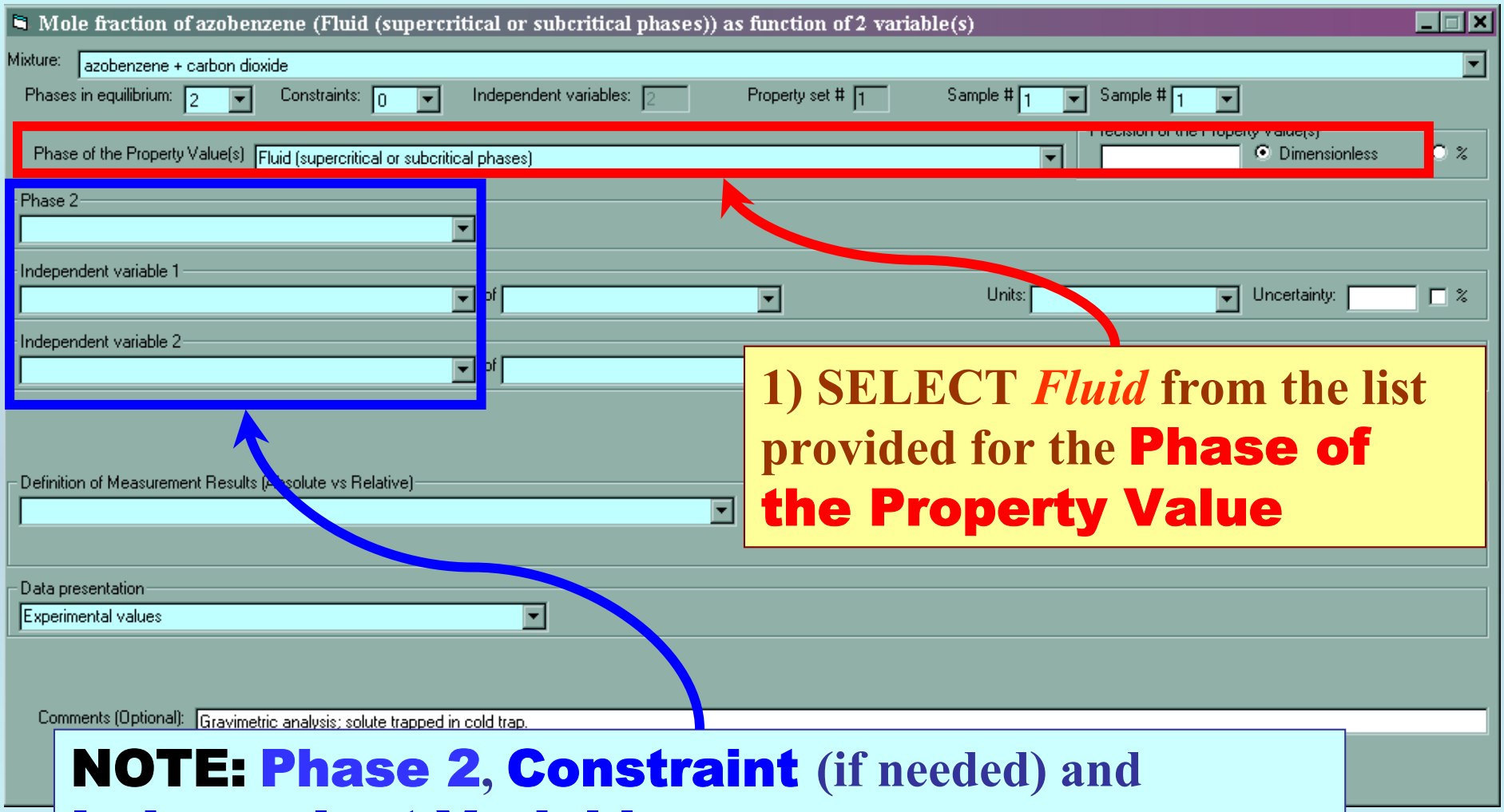
There are 2 here (*crystal* and *fluid*).

Enter the # of Constraints.

There are 0 constraints in the present example.

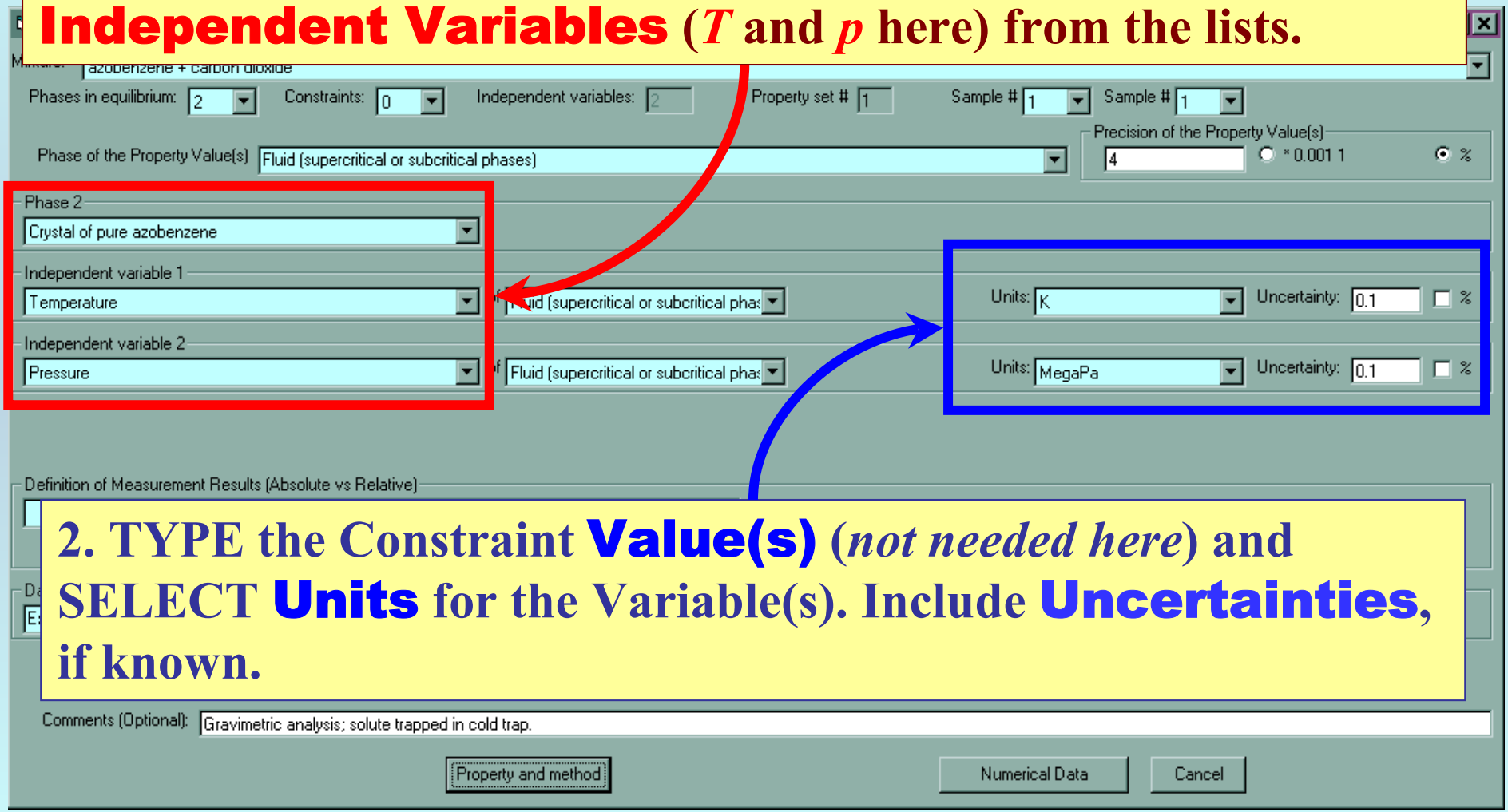
If *T* and/or *p* were held constant, this value would be non-zero.


Mole fraction of azobenzene () (Dimensionless) as function of 2 variable(s)
Mixture:
azobenzene + carbon dioxide
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
Dimensionless
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Gravimetric analysis; solute trapped in cold trap.
Property and method
Numerical Data
Cancel


Mole fraction of azobenzene (Fluid (supercritical or subcritical phases)) as function of 2 variable(s)
Mixture:
azobenzene + carbon dioxide
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Fluid (supercritical or subcritical phases)
Dimensionless
%
Phase 2
Independent variable 1
Units:
Uncertainty:
%
Independent variable 2
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Gravimetric analysis; solute trapped in cold trap.
1) SELECT Fluid from the list provided for the Phase of the Property Value
NOTE: Phase 2, Constraint (if needed) and Independent Variable field(s) appear automatically based on the entries and the Gibbs Phase Rule.

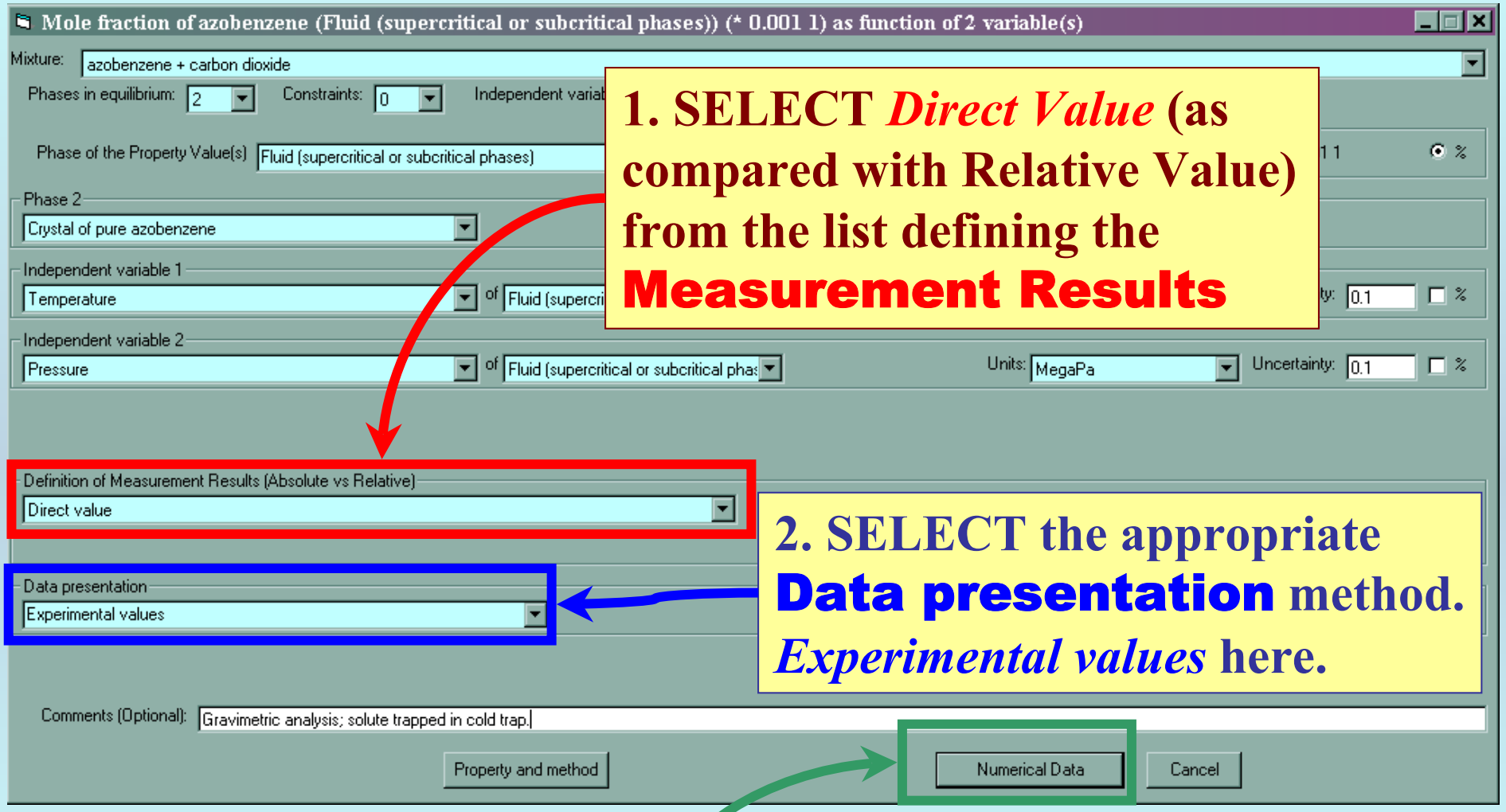
Specification of constraints, constraint values, and constraint units

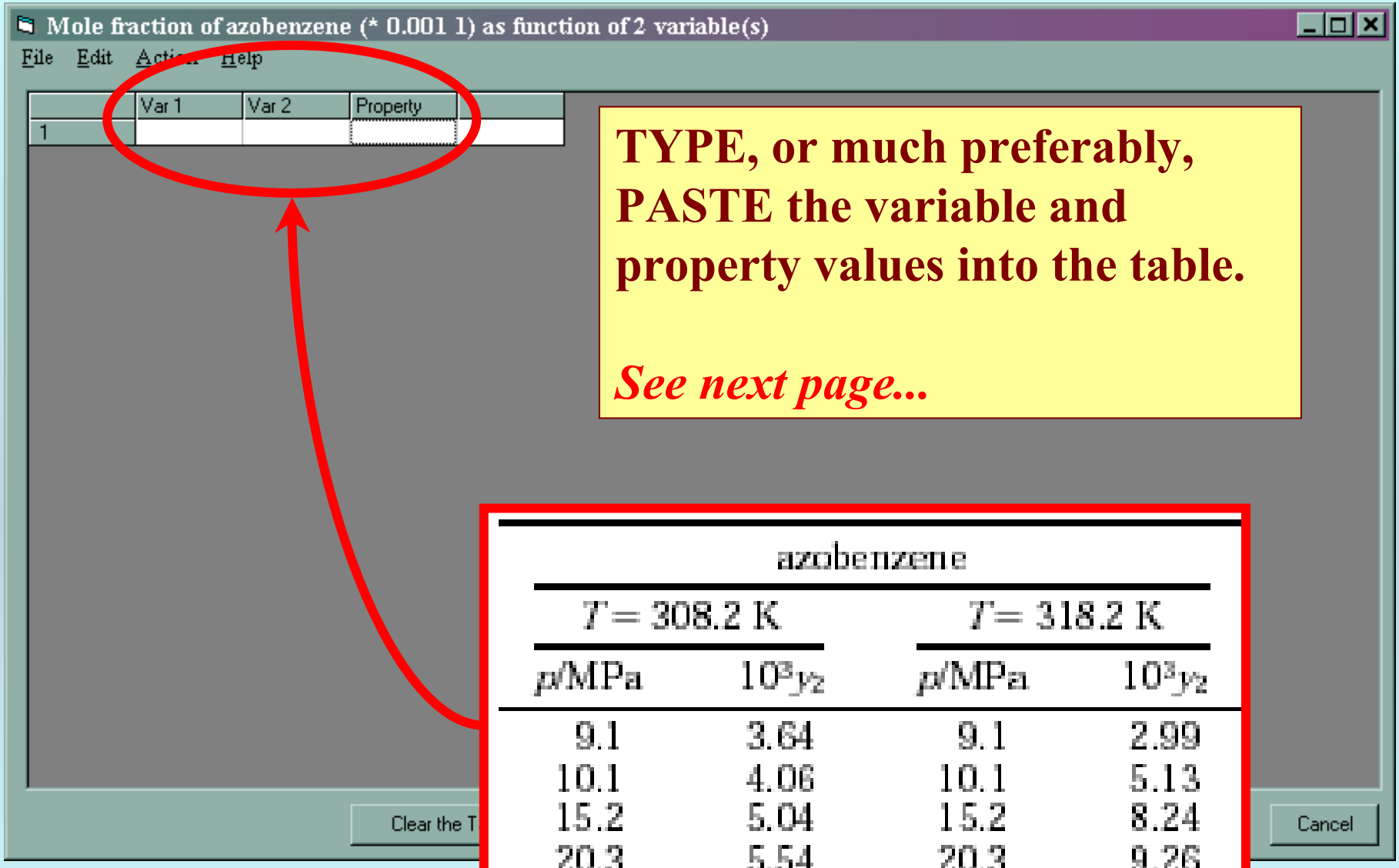
1. SELECT the Constraints (*not needed in this example*), Phase 2 (*Crystal of pure azobenzene* here) and the Independent Variables (*T* and *p* here) from the lists.



2. TYPE the Constraint Value(s) (*not needed here*) and SELECT Units for the Variable(s). Include Uncertainties, if known.

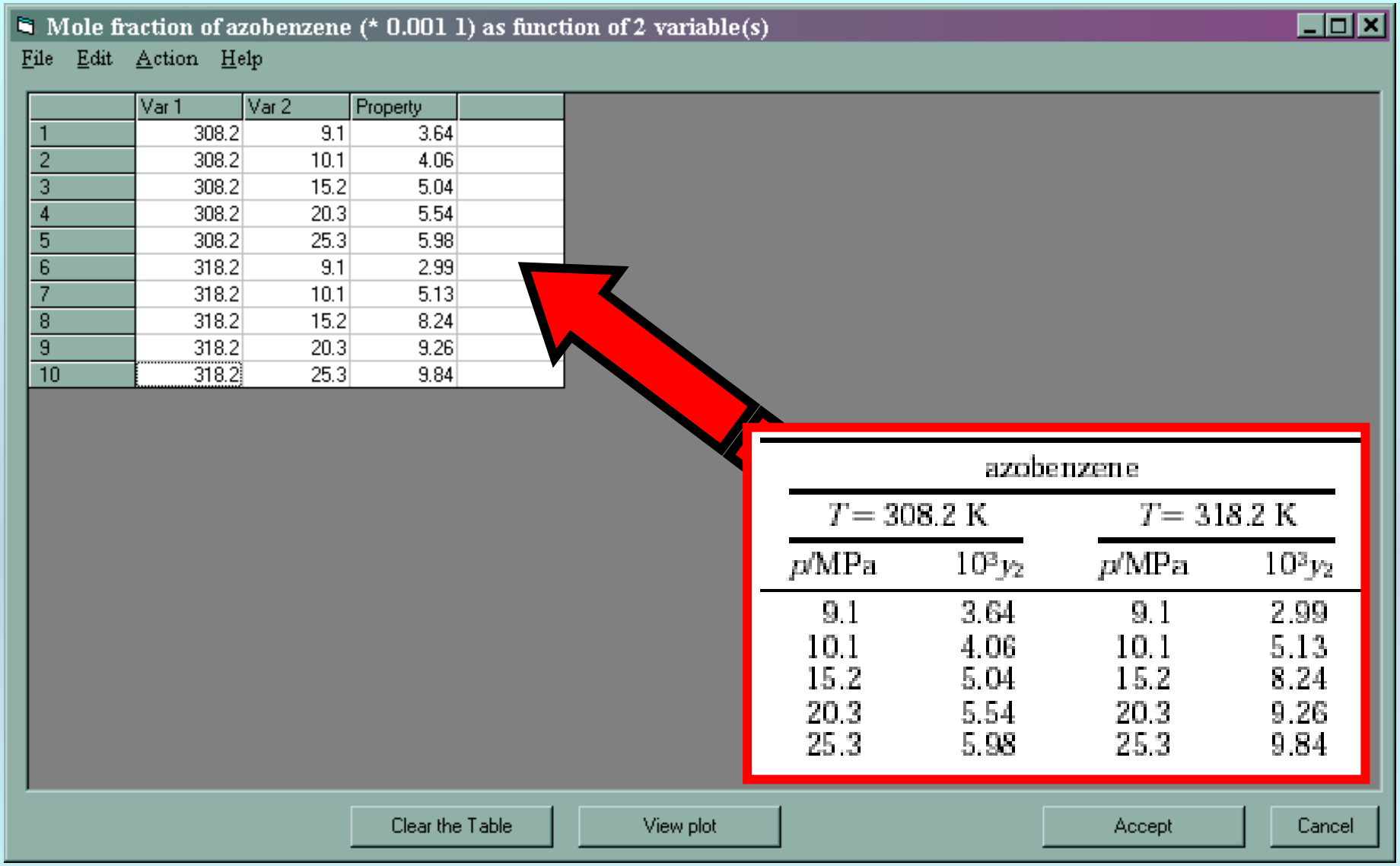
Measurement definition and Data presentation



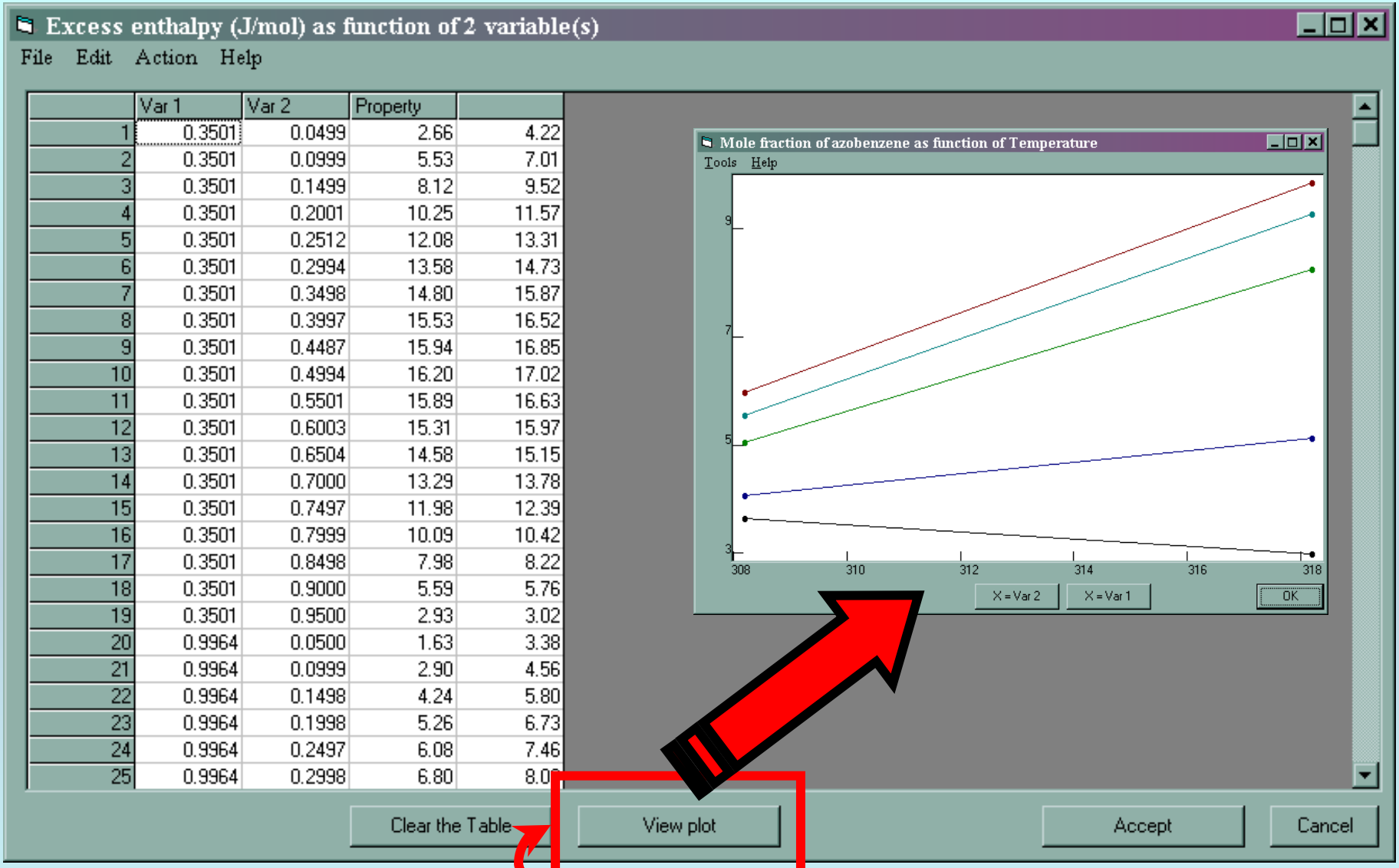


azobenzene

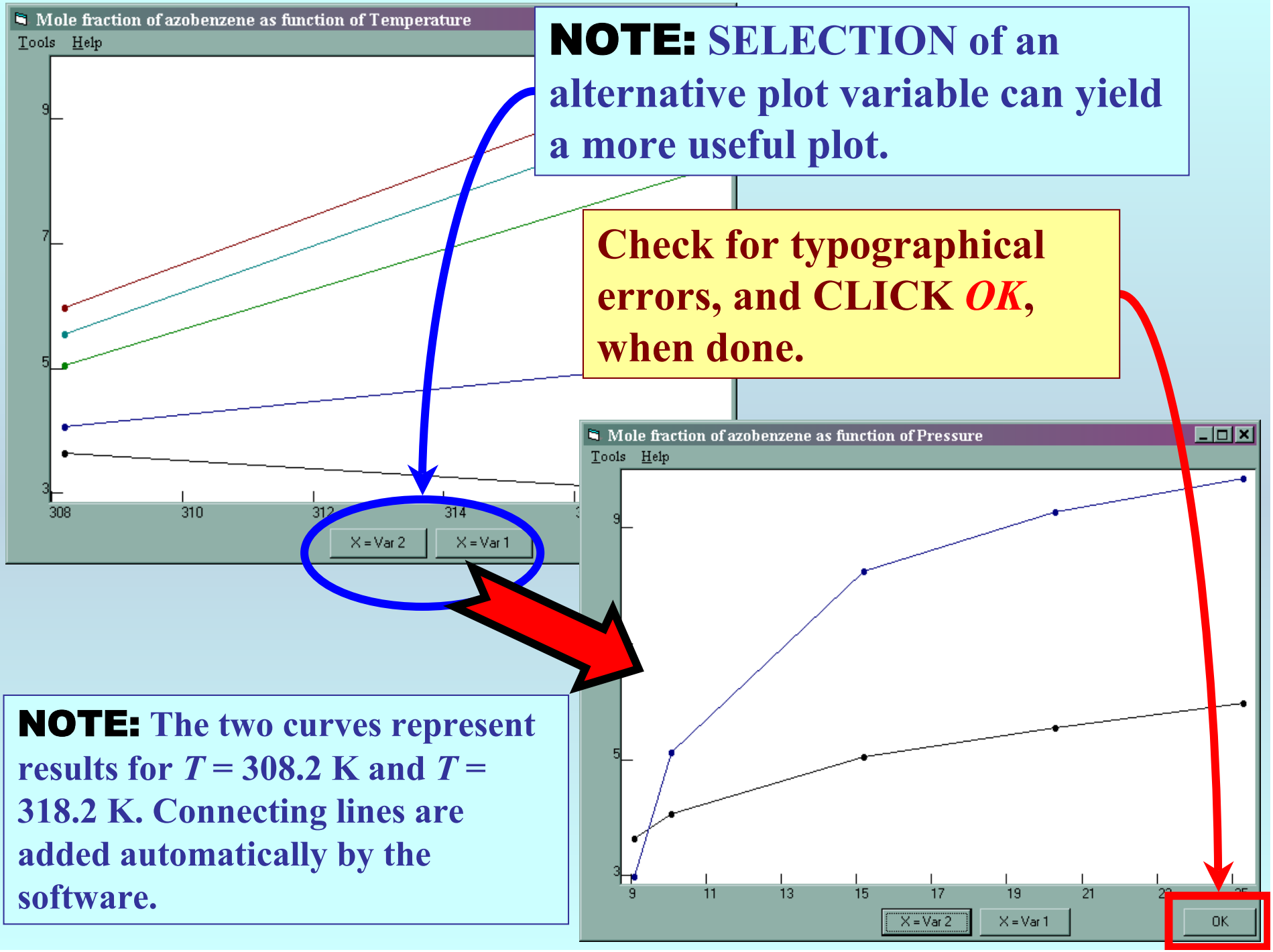
$T = 308.2$ K		$T = 318.2$ K	
p/MPa	$10^3 y_2$	p/MPa	$10^3 y_2$
9.1	3.64	9.1	2.99
10.1	4.06	10.1	5.13
15.2	5.04	15.2	8.24
20.3	5.54	20.3	9.26
25.3	5.98	25.3	9.84

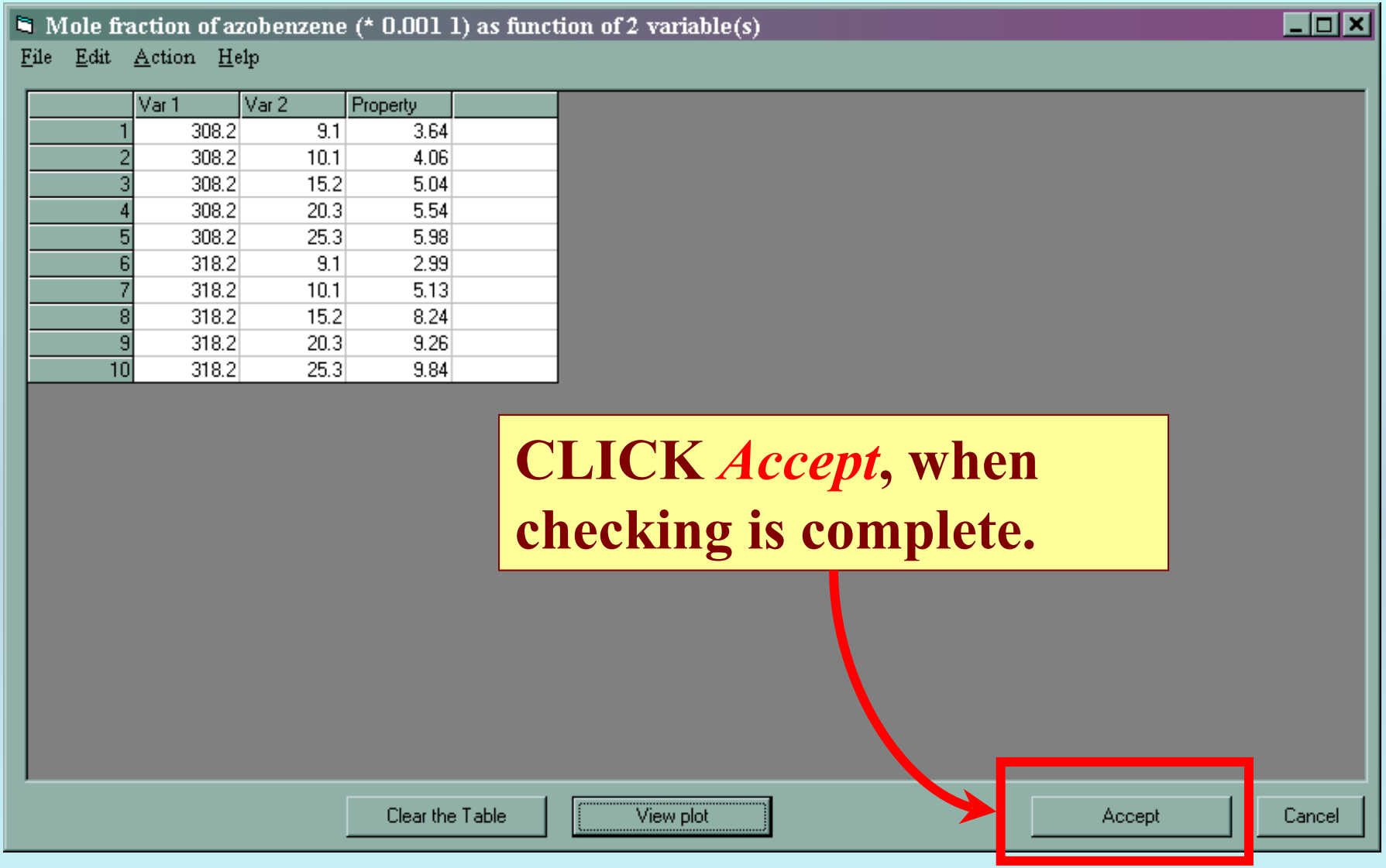


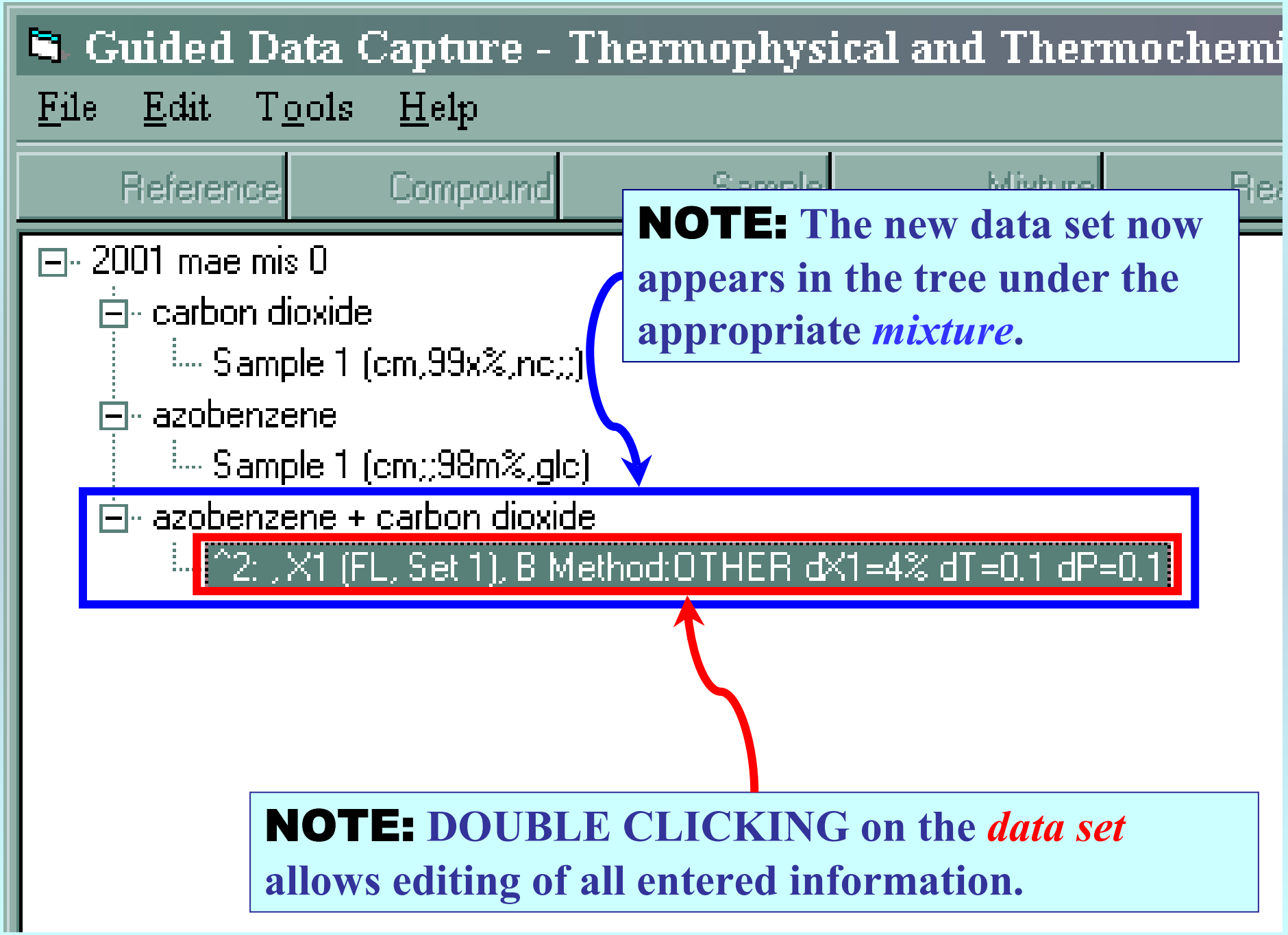
NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)



CLICK *View plot* to see an automatic graphical representation of the data. *NOT very helpful in this case!* See next page...


Mole fraction of azobenzene as function of Temperature
Tools Help
9
7
5
3
308
310
312
314
X = Var 2
X = Var 1
NOTE: SELECTION of an alternative plot variable can yield a more useful plot.
Check for typographical errors, and CLICK OK, when done.
Mole fraction of azobenzene as function of Pressure
Tools Help
9
5
3
9
11
13
15
17
19
21
X = Var 2
X = Var 1
OK
NOTE: The two curves represent results for T = 308.2 K and T = 318.2 K. Connecting lines are added automatically by the software.


Mole fraction of azobenzene (* 0.001 1) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 308.2 9.1 3.64
2 308.2 10.1 4.06
3 308.2 15.2 5.04
4 308.2 20.3 5.54
5 308.2 25.3 5.98
6 318.2 9.1 2.99
7 318.2 10.1 5.13
8 318.2 15.2 8.24
9 318.2 20.3 9.26
10 318.2 25.3 9.84
CLICK Accept, when checking is complete.
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemi
File Edit Tools Help
Reference
Compound
2001 mae mis 0
carbon dioxide
Sample 1 (cm,99x%,nc;;)
azobenzene
Sample 1 (cm;;98m%,glc)
azobenzene + carbon dioxide
^2: ,X1 (FL, Set 1), B Method:OTHER dX1=4% dT=0.1 dP=0.1
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.**