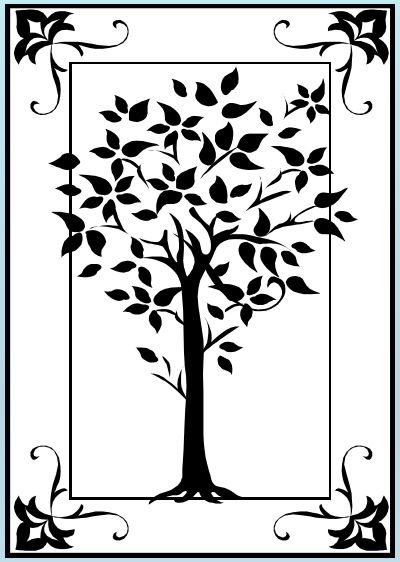
METADATA AND NUMERICAL DATA CAPTURE:
SOLUBILITY (composition)
(2 – Components: Liquid & Gas)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components: Liquid & Gas**
SOLUBILITIES (composition)
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:

784 *J. Chem. Eng. Data* 1999, *44*, 784−787

Solubilities of Nitrogen in Heavy Normal Paraffins from 323 to 423 K at Pressures to 18.0 MPa

Jianfen Tong, Wuzi Gao, Robert L. Robinson, Jr.,* and Khaled A. M. Gasem

School of Chemical Engineering, Oklahoma State University, Stillwater, Oklahoma 74078-0537

The solubilities of nitrogen in selected *n*-paraffin hydrocarbons (decane, eicosane, octacosane, hexatriacontane) were measured using a static equilibrium cell over the temperature range from 323.2 to 423.2 K at pressures to 18.0 MPa. The uncertainty in the measured solubilities is estimated to be less than 0.001 in mole fraction. The data were analyzed using the Soave−Redlich−Kwong (SRK) and Peng−Robinson (PR) equations of state. In general, the two equations represent the experimental data well when a single interaction parameter C_{ij} is used for each binary system. The data display a trend of increasing solubility of nitrogen with increased temperature, pressure, and *n*-paraffin chain length.

SOLUBILITY (composition)

(2 ñ Components: Liquid & Gas)

Nitrogen + Decane

Table 1. Solubility of Nitrogen in *n*-Paraffin Hydrocarbons

x_1	p/MPa	x_1	p/MPa
	Decane		
	344.3 K		
0.0556	4.33	0.1178	9.84
0.0590	4.61	0.1202	10.06
0.0633	4.97	0.1539	13.40
0.1087	8.99	0.1578	13.81
	377.6 K		
0.0568	4.05	0.1662	13.15
0.0689	4.97	0.1708	13.63
0.1158	8.73	0.1967	16.04
0.1271	9.66		
	410.9 K		
0.0598	3.91	0.1343	9.25
0.0749	4.92	0.1690	11.99
0.1162	7.89	0.1894	13.61

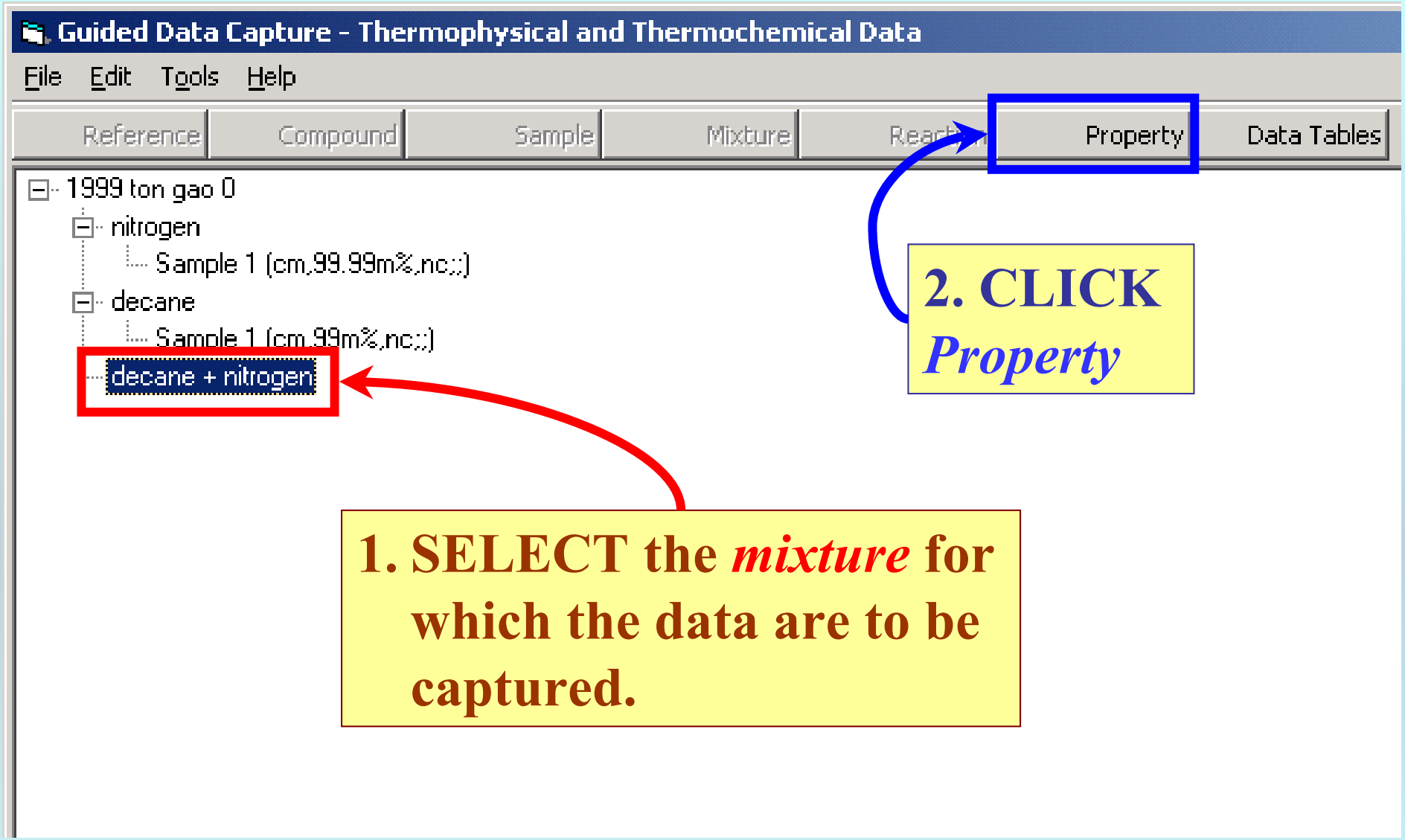
This data set is considered here.

Experimental Method Info:

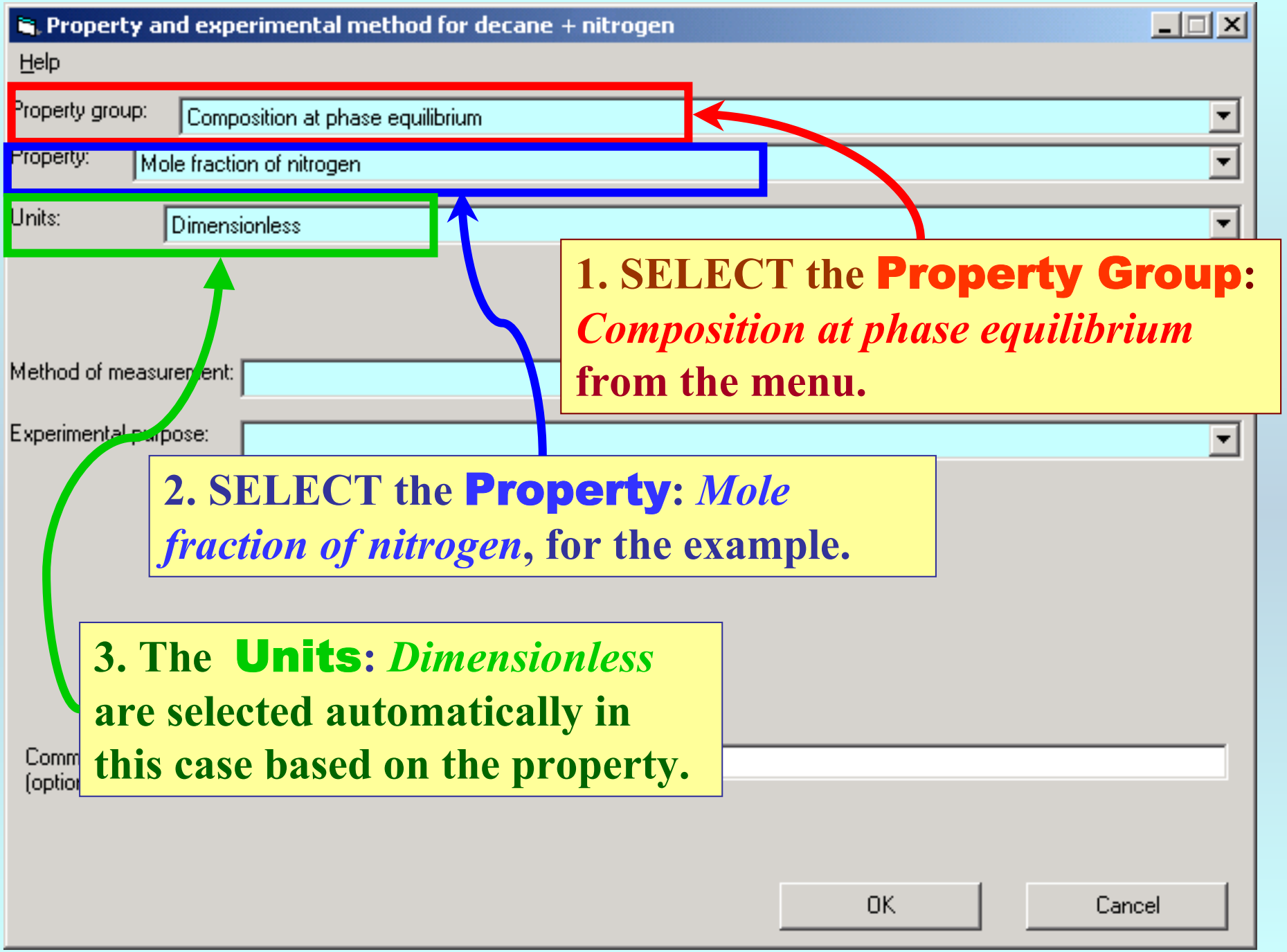
Experimental Method

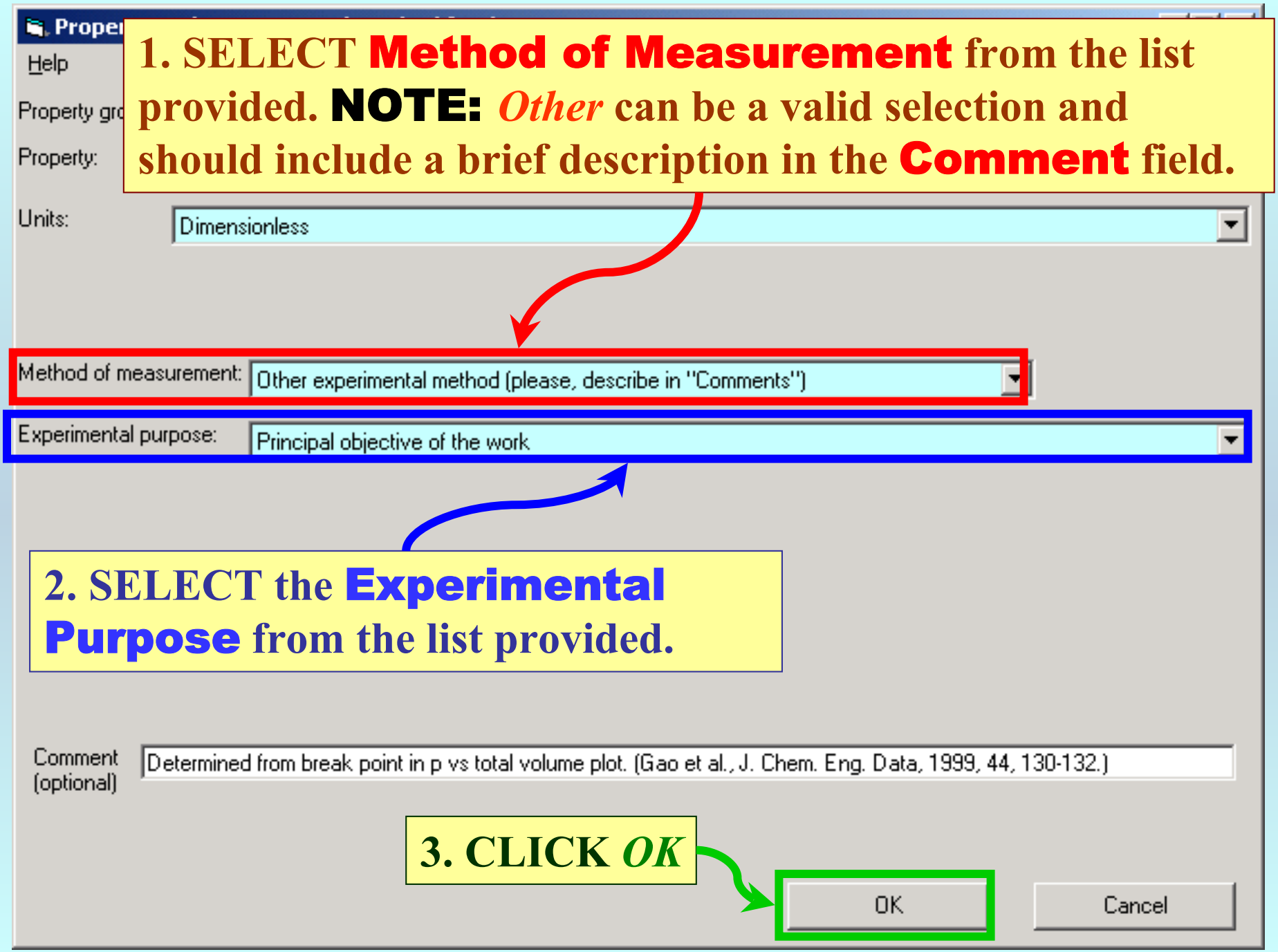
A variable-volume, static-type blind equilibrium cell was used in this study. The apparatus and procedures have been described previously (Gao et al., 1999b). The measurement uncertainties are estimated to be 0.1 K in temperature and less than 0.001 in mole fraction. The estimated uncertainty in the bubble point pressure is on the order of 0.07 MPa for the systems studied here. A detailed error analysis is given by Darwish (1991).

Gao, W.; Gasem, K. A. M.; Robinson, R. L., Jr. High-Pressure Solubilities of Hydrogen, Nitrogen and Carbon Monoxide in Dodecane from 344 to 410 K at Pressures to 13.2 MPa. *J. Chem. Eng. Data* **1999b**, *44*, 130−132.



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 decane + nitrogen
Help
Property group:
Composition at phase equilibrium
Property:
Mole fraction of nitrogen
Units:
Dimensionless
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Composition at phase equilibrium from the menu.
2. SELECT the Property: Mole fraction of nitrogen, for the example.
3. The Units: Dimensionless are selected automatically in this case based on the property.
OK
Cancel

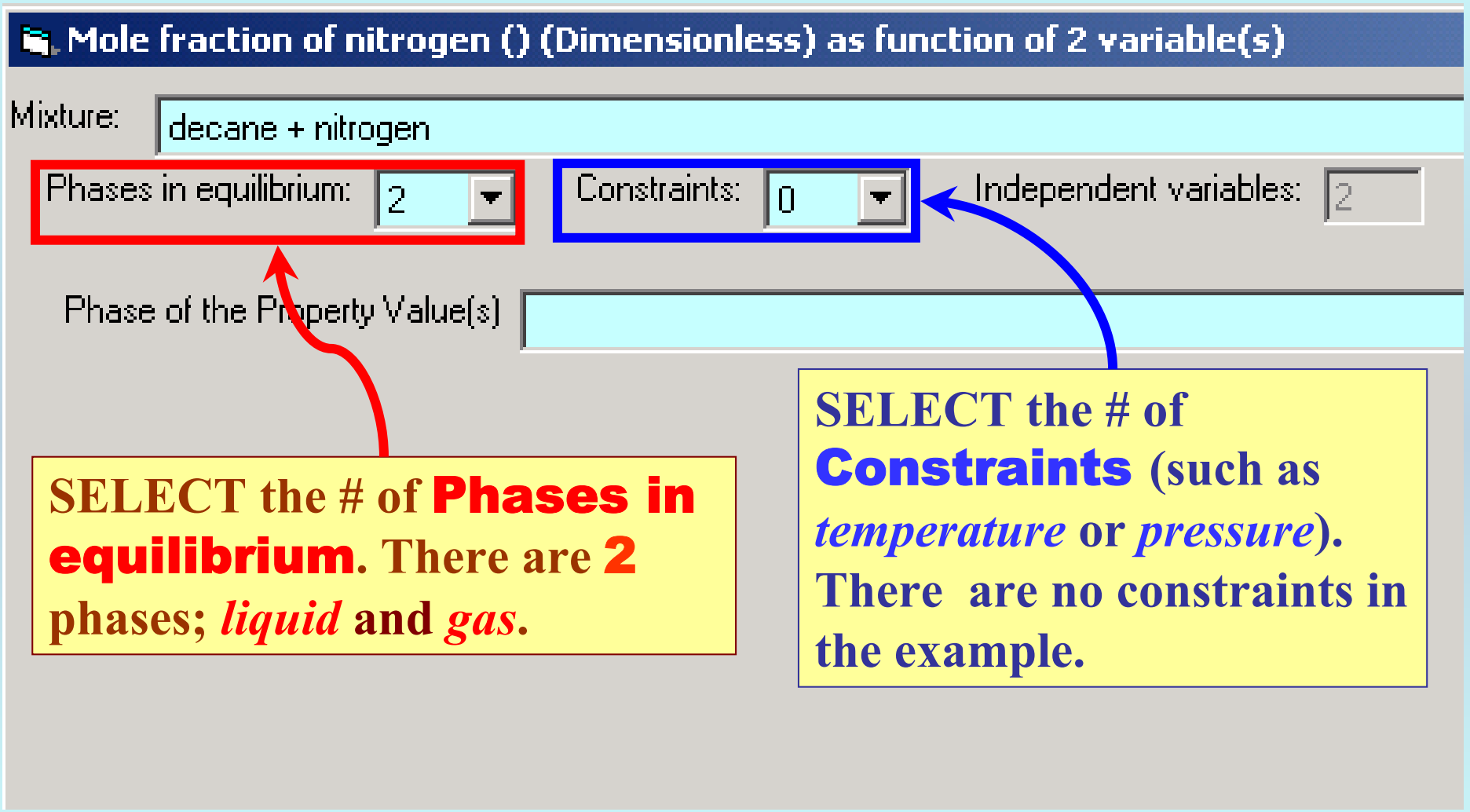


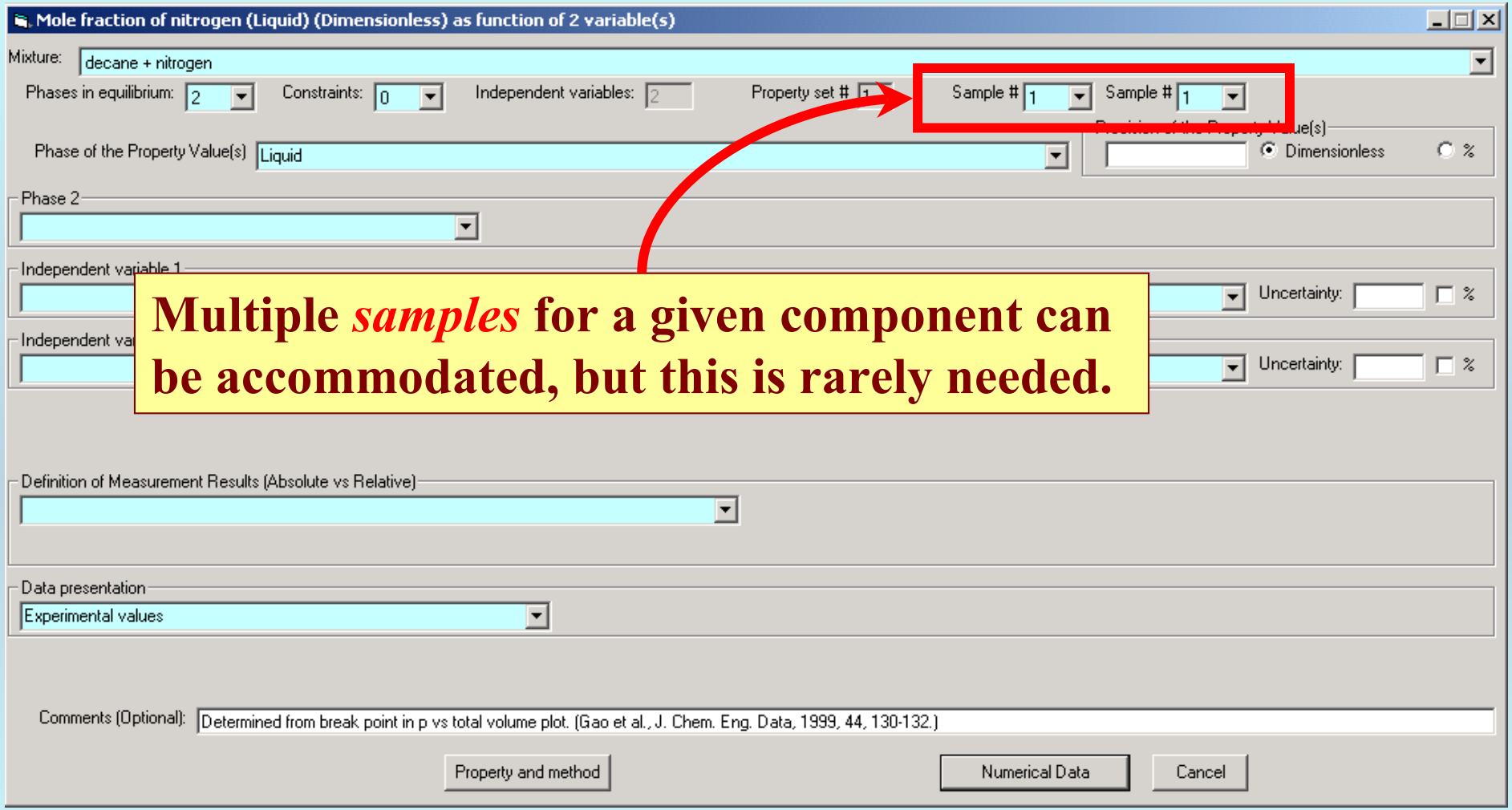
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

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

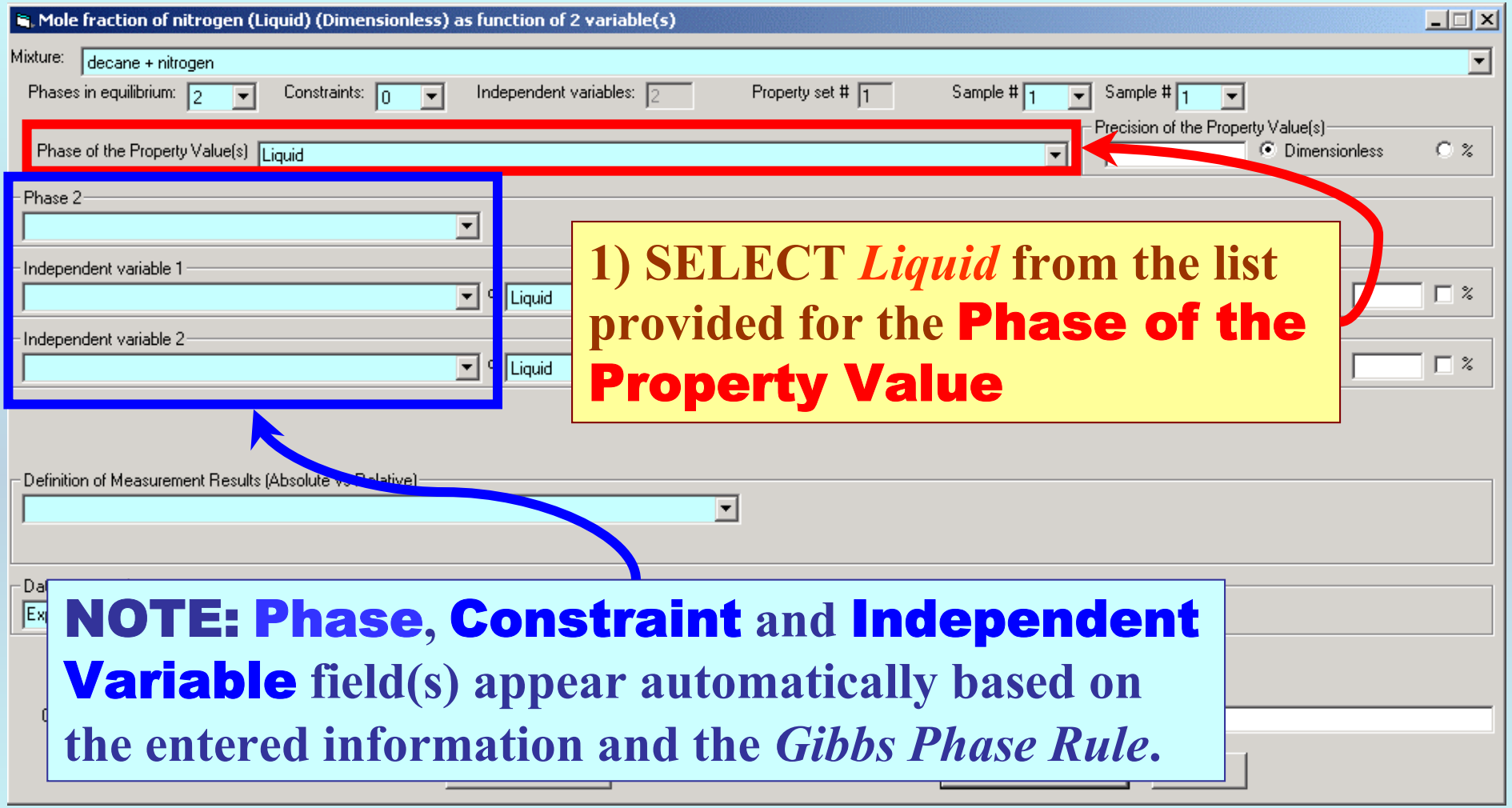
3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints

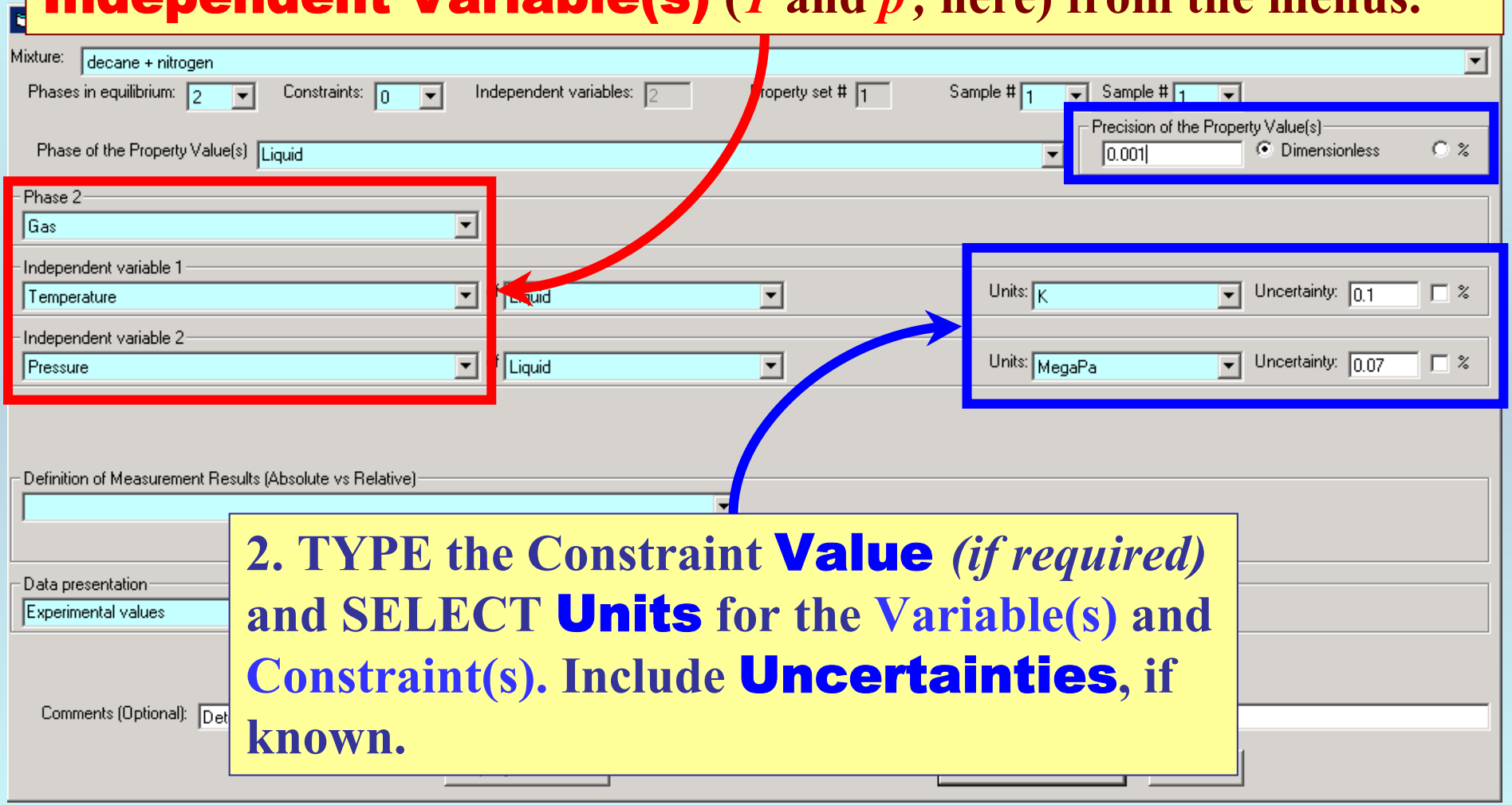




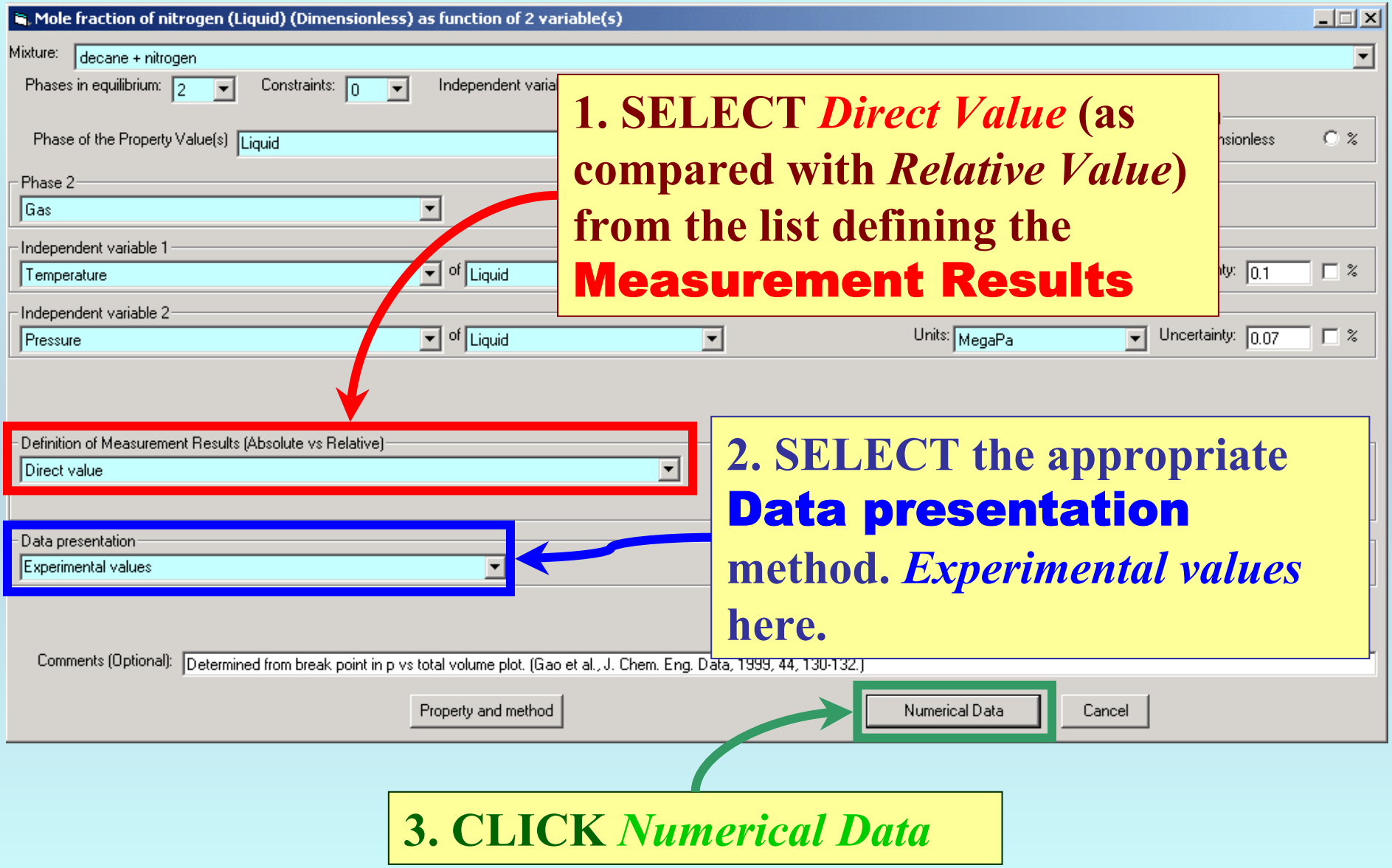
Multiple *samples* for a given component can be accommodated, but this is rarely needed.

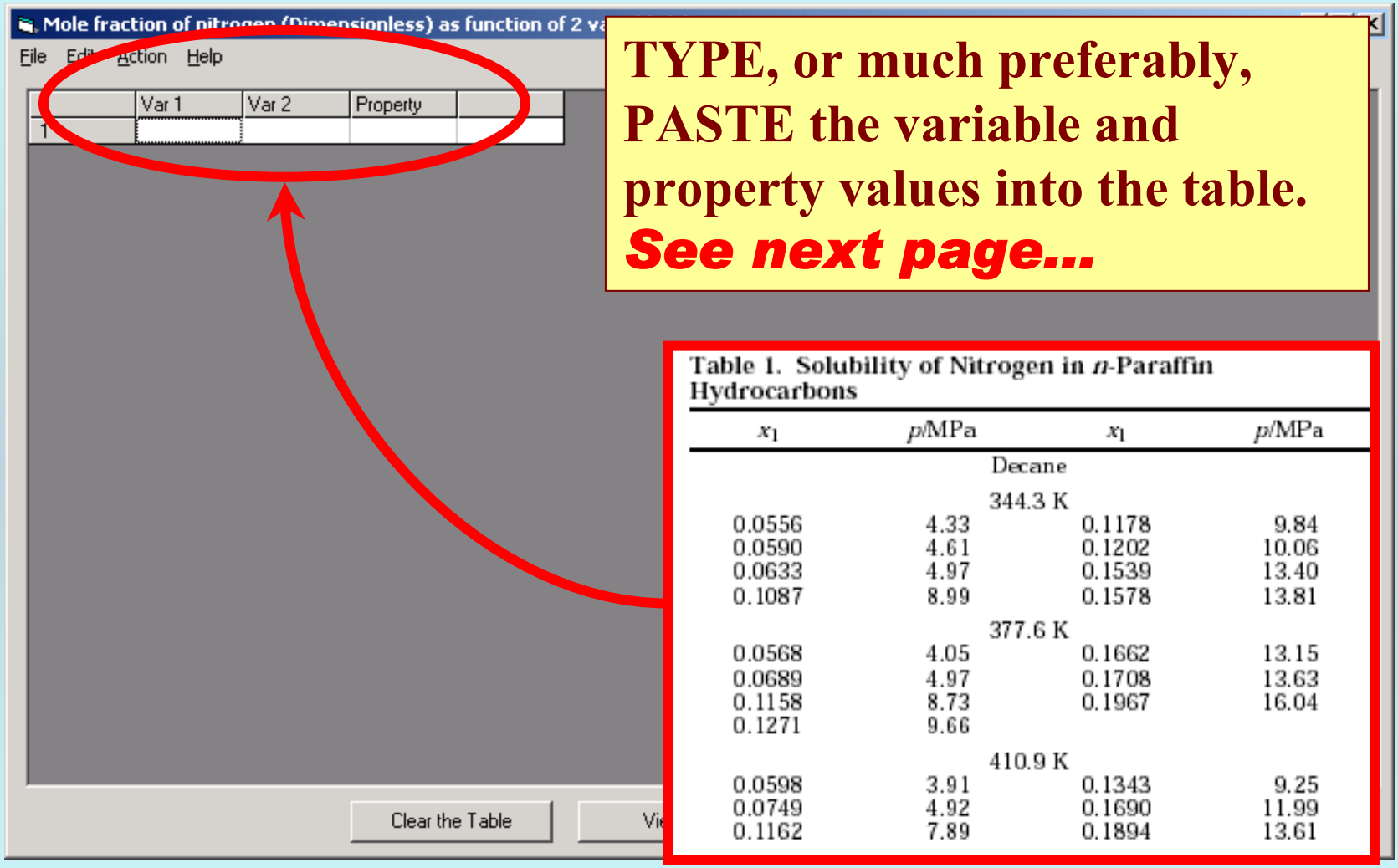

Mole fraction of nitrogen (Liquid) (Dimensionless) as function of 2 variable(s)
Mixture:
decane + nitrogen
Phases in equilibrium:
2
Constraints:
0
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
Dimensionless
%
Phase 2
Independent variable 1
Liquid
Independent variable 2
Liquid
Definition of Measurement Results (Absolute vs. Relative)
1) SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Phase, Constraint and Independent Variable field(s) appear automatically based on the entered information and the Gibbs Phase Rule.

1. SELECT **Phase 2** (*gas*), **Constraint(s)** (none here) and the **Independent Variable(s)** (*T* and *p*, here) from the menus.



2. TYPE the Constraint **Value** *(if required)* and SELECT **Units** for the Variable(s) and Constraint(s). Include **Uncertainties**, if known.


Mole fraction of nitrogen (Liquid) (Dimensionless) as function of 2 variable(s)
Mixture: decane + nitrogen
Phases in equilibrium: 2
Constraints: 0
Phase of the Property Value(s): Liquid
Phase 2
Gas
Independent variable 1
Temperature
of Liquid
Independent variable 2
Pressure
of Liquid
Units: MegaPa
Uncertainty: 0.07
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional): Determined from break point in p vs total volume plot. (Gao et al., J. Chem. Eng. Data, 1999, 44, 130-132.)
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

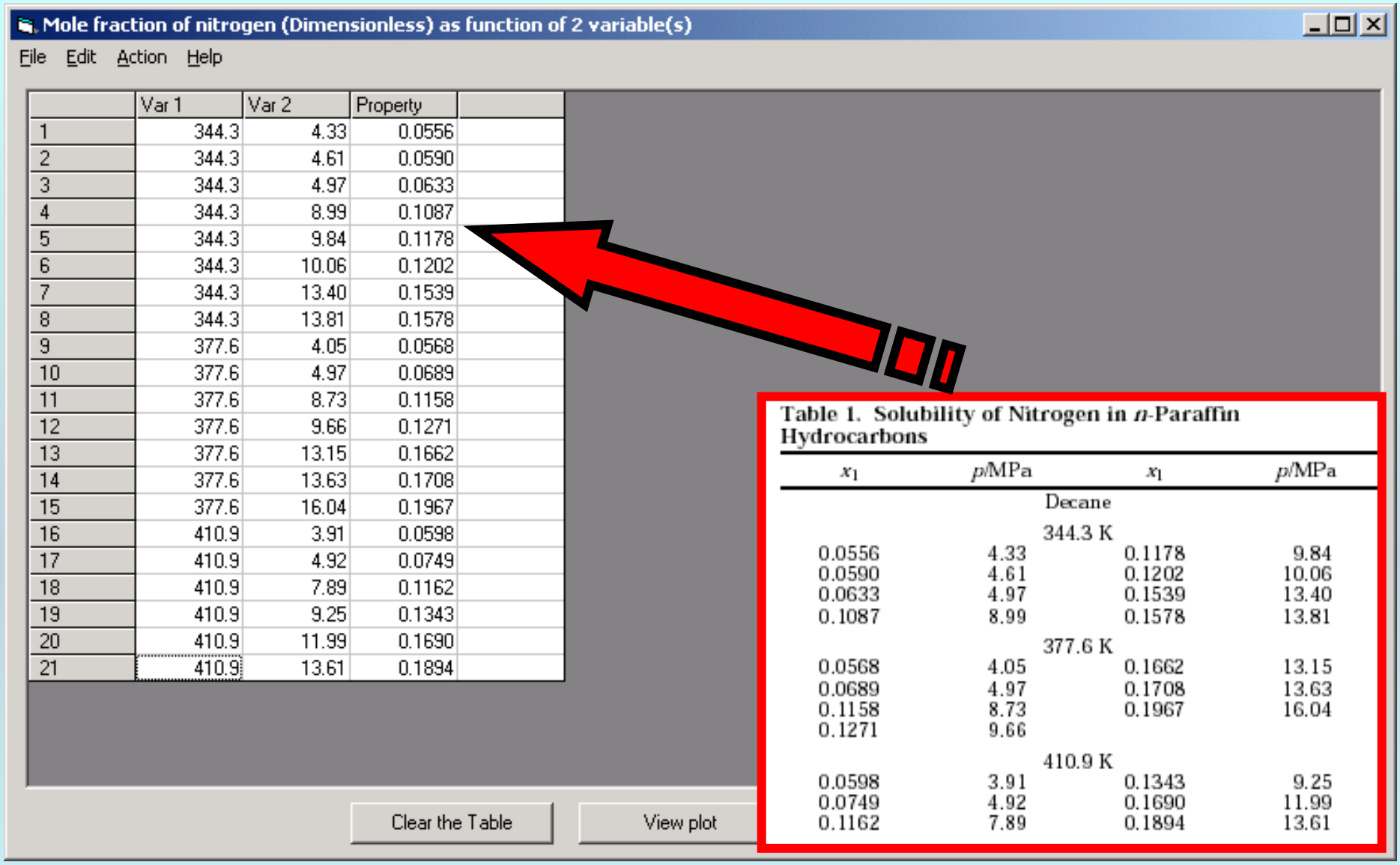


TYPE, or much preferably, PASTE the variable and property values into the table.

See next page...

Table 1. Solubility of Nitrogen in *n*-Paraffin Hydrocarbons

x_1	p/MPa	x_1	p/MPa
	Decane		
	344.3 K		
0.0556	4.33	0.1178	9.84
0.0590	4.61	0.1202	10.06
0.0633	4.97	0.1539	13.40
0.1087	8.99	0.1578	13.81
	377.6 K		
0.0568	4.05	0.1662	13.15
0.0689	4.97	0.1708	13.63
0.1158	8.73	0.1967	16.04
0.1271	9.66		
	410.9 K		
0.0598	3.91	0.1343	9.25
0.0749	4.92	0.1690	11.99
0.1162	7.89	0.1894	13.61



	Var 1	Var 2	Property
1	344.3	4.33	0.0556
2	344.3	4.61	0.0590
3	344.3	4.97	0.0633
4	344.3	8.99	0.1087
5	344.3	9.84	0.1178
6	344.3	10.06	0.1202
7	344.3	13.40	0.1539
8	344.3	13.81	0.1578
9	377.6	4.05	0.0568
10	377.6	4.97	0.0689
11	377.6	8.73	0.1158
12	377.6	9.66	0.1271
13	377.6	13.15	0.1662
14	377.6	13.63	0.1708
15	377.6	16.04	0.1967
16	410.9	3.91	0.0598
17	410.9	4.92	0.0749
18	410.9	7.89	0.1162
19	410.9	9.25	0.1343
20	410.9	11.99	0.1690
21	410.9	13.61	0.1894

Table 1. Solubility of Nitrogen in *n*-Paraffin Hydrocarbons

x_1	p/MPa	x_1	p/MPa
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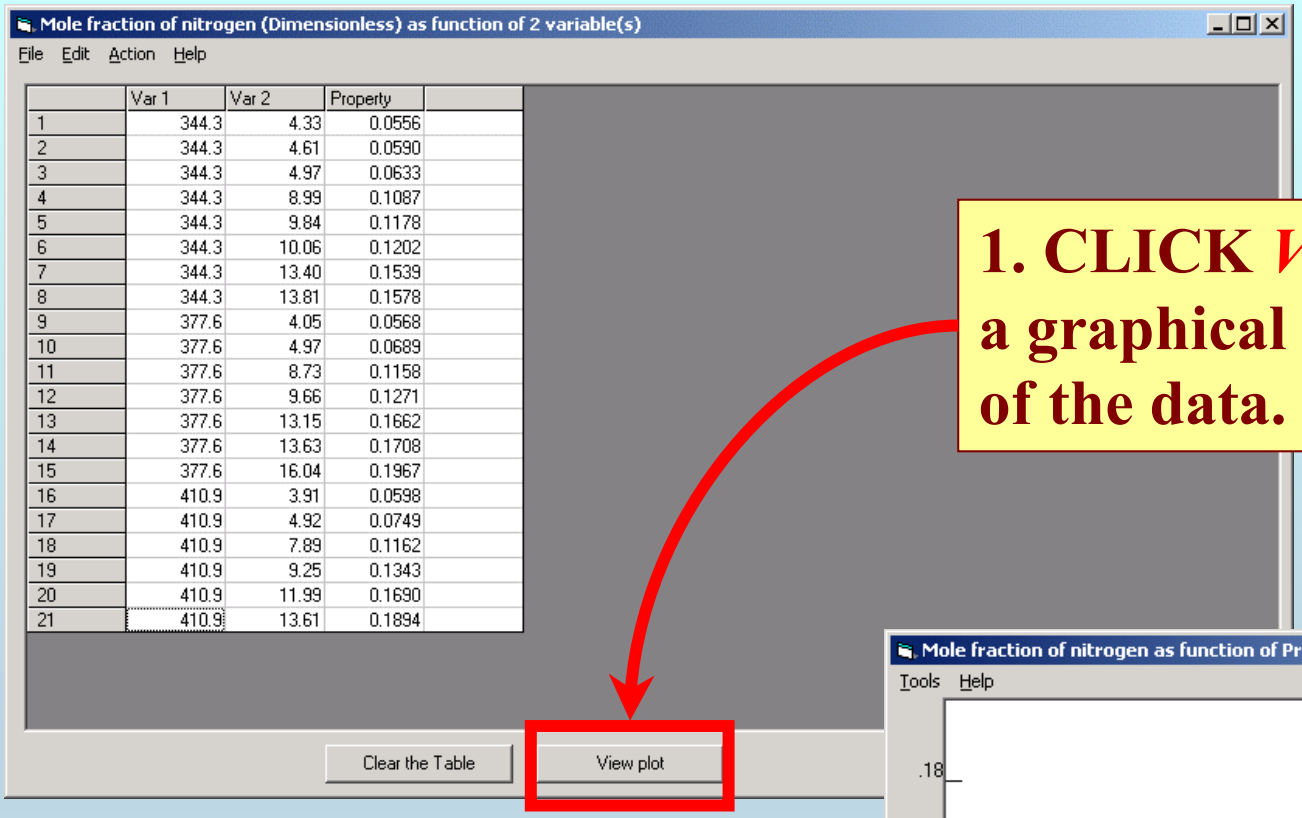
0.0749	4.92	0.1690	11.99
0.1162	7.89	0.1894	13.61

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.)



	Var 1	Var 2	Property
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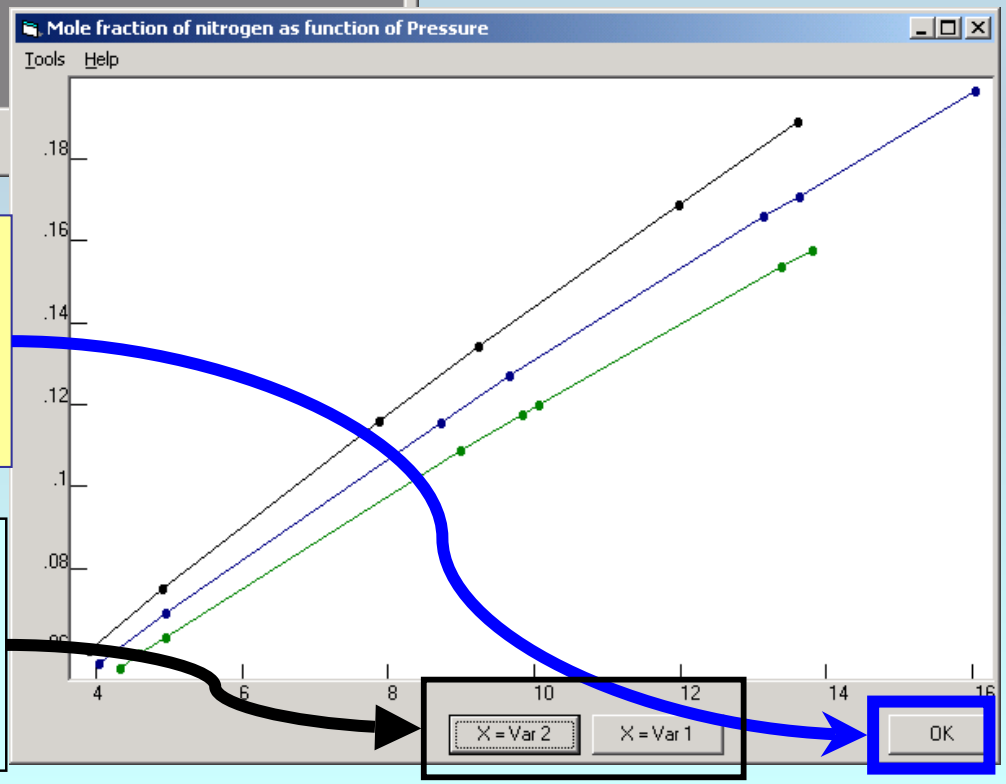
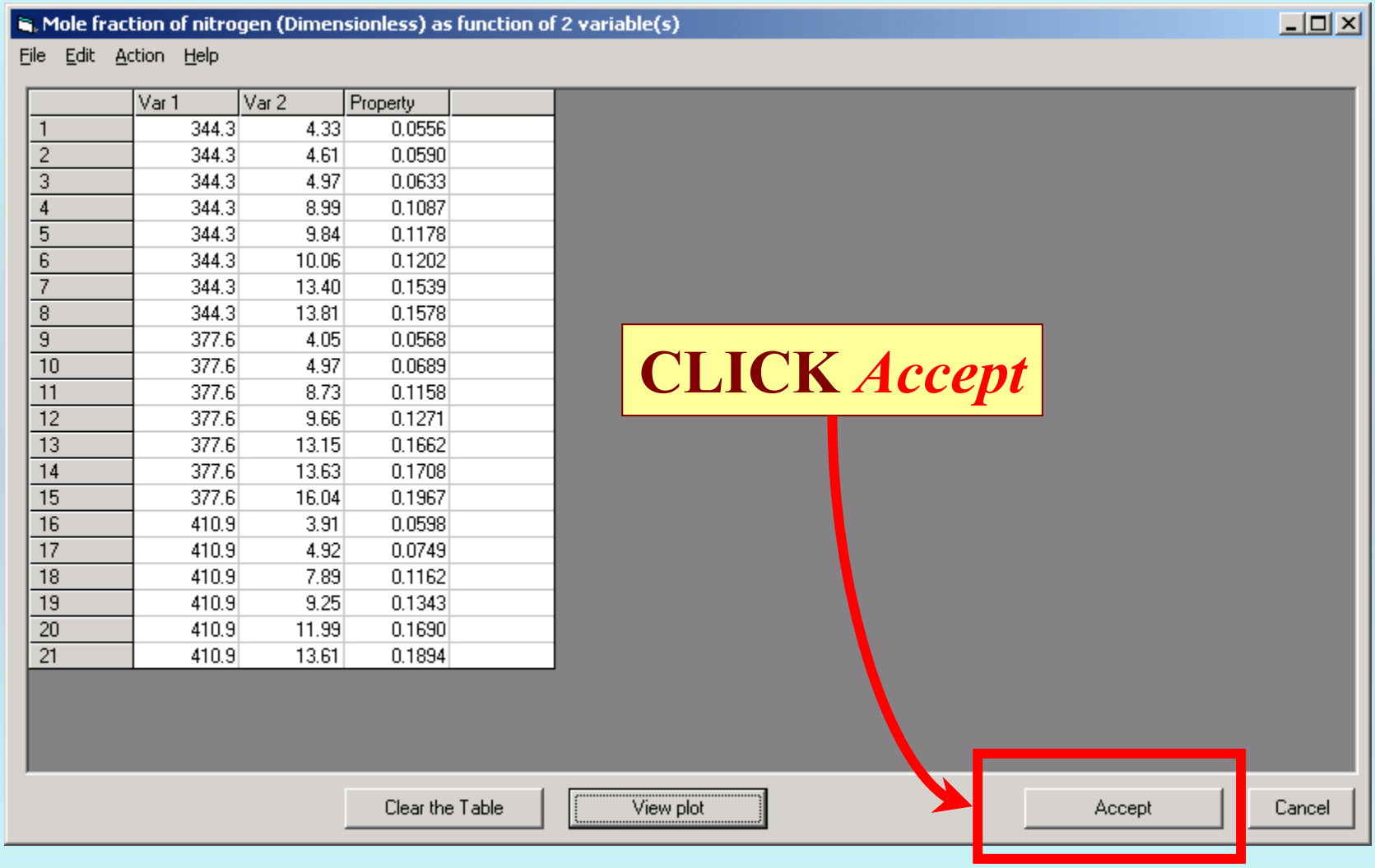
16	410.9	3.91	0.0598
17	410.9	4.92	0.0749
18	410.9	7.89	0.1162
19	410.9	9.25	0.1343
20	410.9	11.99	0.1690
21	410.9	13.61	0.1894

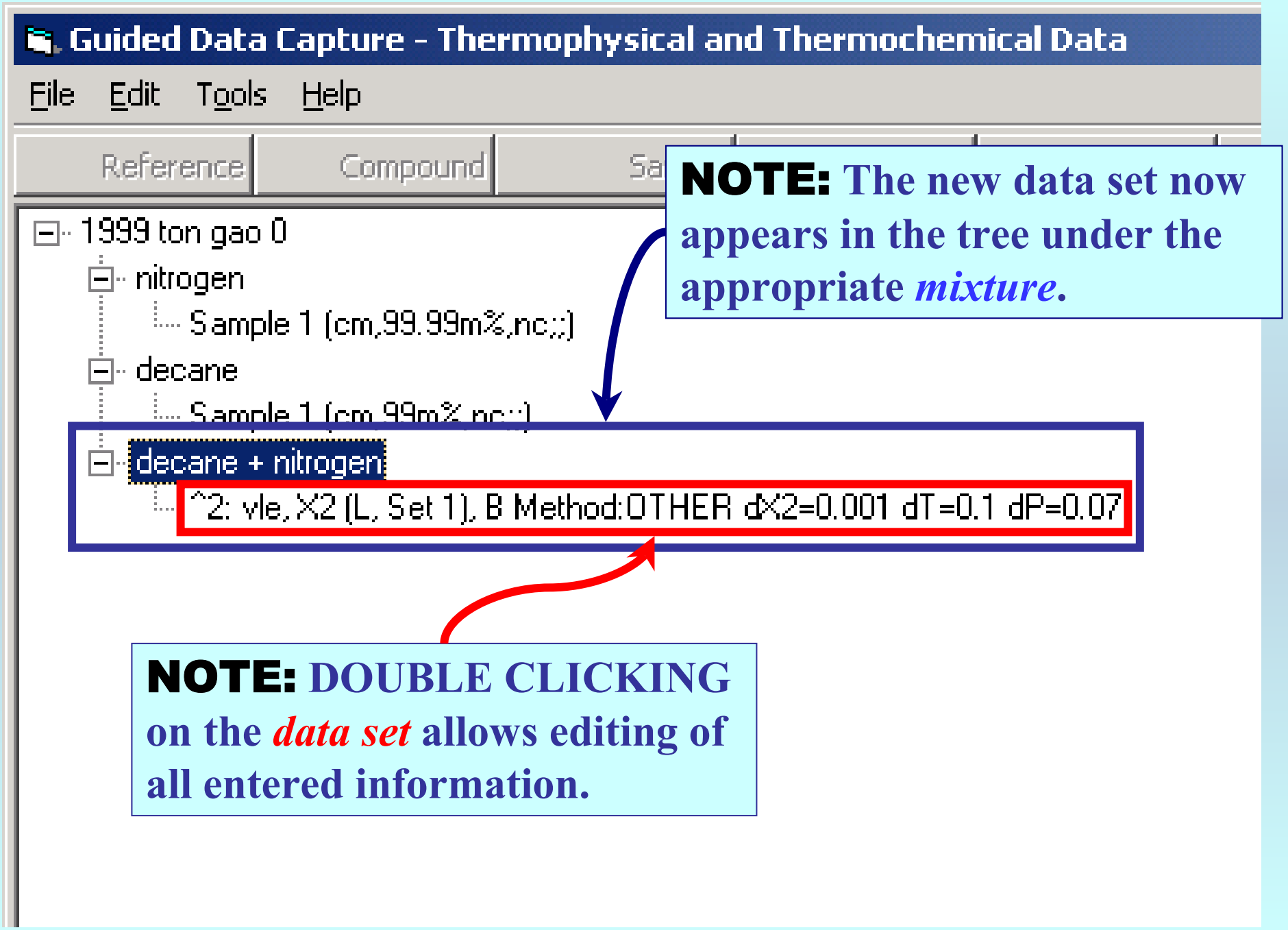
1. CLICK *View plot* to see a graphical representation of the data.



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

NOTE: The variable associated with the x-axis can be selected for best display.


Mole fraction of nitrogen (Dimensionless) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 344.3 4.33 0.0556
2 344.3 4.61 0.0590
3 344.3 4.97 0.0633
4 344.3 8.99 0.1087
5 344.3 9.84 0.1178
6 344.3 10.06 0.1202
7 344.3 13.40 0.1539
8 344.3 13.81 0.1578
9 377.6 4.05 0.0568
10 377.6 4.97 0.0689
11 377.6 8.73 0.1158
12 377.6 9.66 0.1271
13 377.6 13.15 0.1662
14 377.6 13.63 0.1708
15 377.6 16.04 0.1967
16 410.9 3.91 0.0598
17 410.9 4.92 0.0749
18 410.9 7.89 0.1162
19 410.9 9.25 0.1343
20 410.9 11.99 0.1690
21 410.9 13.61 0.1894
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
1999 ton gao 0
nitrogen
Sample 1 (cm,99.99m%,nc;;)
decane
decane + nitrogen
^2: vle, X2 (L, Set 1), B Method:OTHER dX2=0.001 dT=0.1 dP=0.07
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.**