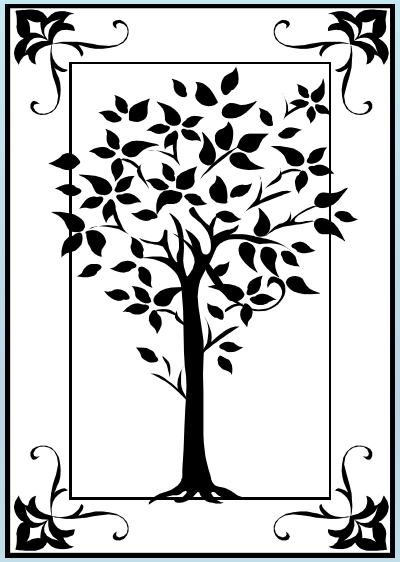
METADATA AND NUMERICAL DATA CAPTURE:
INTERFACIAL TENSION
2 – Components at constant pressure

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components at constant pressure**
INTERFACIAL TENSION ($N \cdot m^{-1}$)
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:

1086 *J. Chem. Eng. Data* 2001, *46*, 1086−1088

Interfacial Tension of Alkane + Water Systems†

Susana Zeppieri, Jhosgre Rodríguez, and A. L. López de Ramos*

Universidad Simón Bolívar, Departamento de Termodinámica y Fenómenos de Transferencia, Grupo de Fenómenos de Transporte (G-10), Apartado Postal 89.000, Caracas 1080-A, Venezuela

Interfacial tension was measured for hexane + water, heptane + water, octane + water, nonane + water, decane + water, undecane + water, and dodecane + water, using the emergent drop experimental technique with a numerical method based on a fourth degree spline interpolation of the drop profile. The experimental equipment used to generate the drop consists of a cell with a stainless steel body and two Pyrex windows. The inner cell was previously filled with water. A surgical needle (at the bottom of the cell) was used to introduce the organic phase into the cell (forming the emergent drop). Water was used to keep the temperature constant inside the cell (between 10 °C and 60 °C). The cell was illuminated from the back using a fiber optic lamp and a diffuser. A video camera (with a 60 mm microlens and an extension ring) was located at the front window. The emergent drop image was captured and sent to the video recording system. The cell and the optical components were placed on an optical table with vibration isolation legs. A new correlation was found to predict interfacial tension (γ) as a function of temperature (t) and the number of carbon atoms (n) with a deviation of less than 0.05% from experimental values.

INTERFACIAL TENSION = f(*T*) with p = 101.3 kPa

(2 ñ Components)

Hexane + Water

Table 1. Interfacial Tension Experimental Values at Different Temperatures

	interfacial tension, γ/mN·m^{-1} ± 0.04				
(t ± 0.1)/°C	hexane + water	heptane + water	octane + water	nonane + water	decane + water
10.0	51.43		52.27	52.69	52.97
15.0	51.11	51.59	52.01	52.37	52.67
20.0	50.80	51.24	51.64	52.06	52.33
25.0	50.38	50.71	51.16	51.63	51.98
27.5	50.11	50.47	51.00	51.48	51.77
30.0	49.96	50.30	50.74	51.21	51.51
32.5	49.70	50.12	50.48	50.95	51.26
35.0	49.44	49.89	50.22	50.68	51.06
37.5	49.18	49.64	50.09	50.54	50.83
40.0	48.92	49.38	49.84	50.27	50.53
45.0	48.52	49.00	49.45	49.87	50.13
50.0	48.13	48.55	48.95	49.36	49.78
55.0			48.58	49.09	49.45
60.0			48.32	48.82	49.21

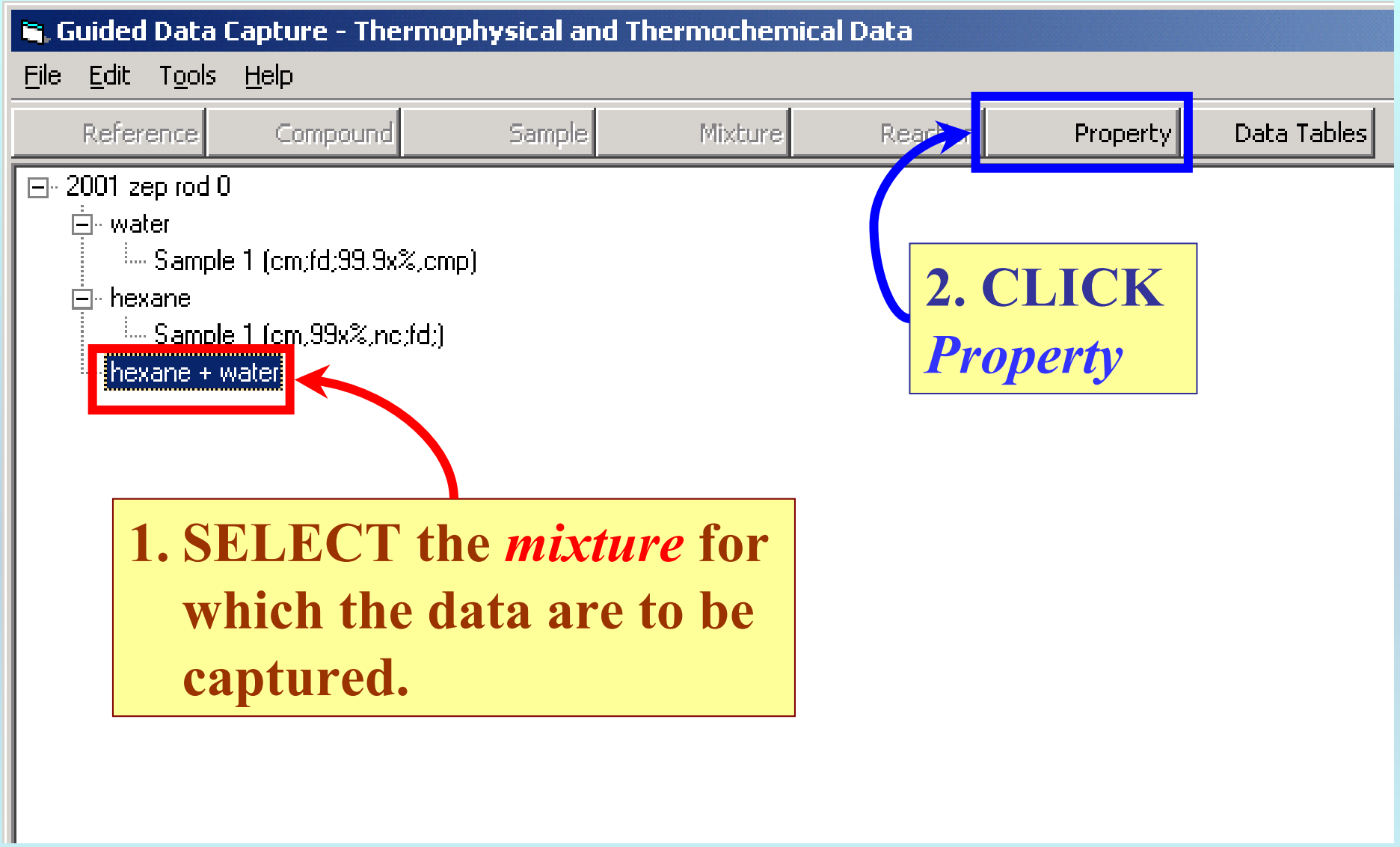
These data are considered here.

Experimental Method Info:

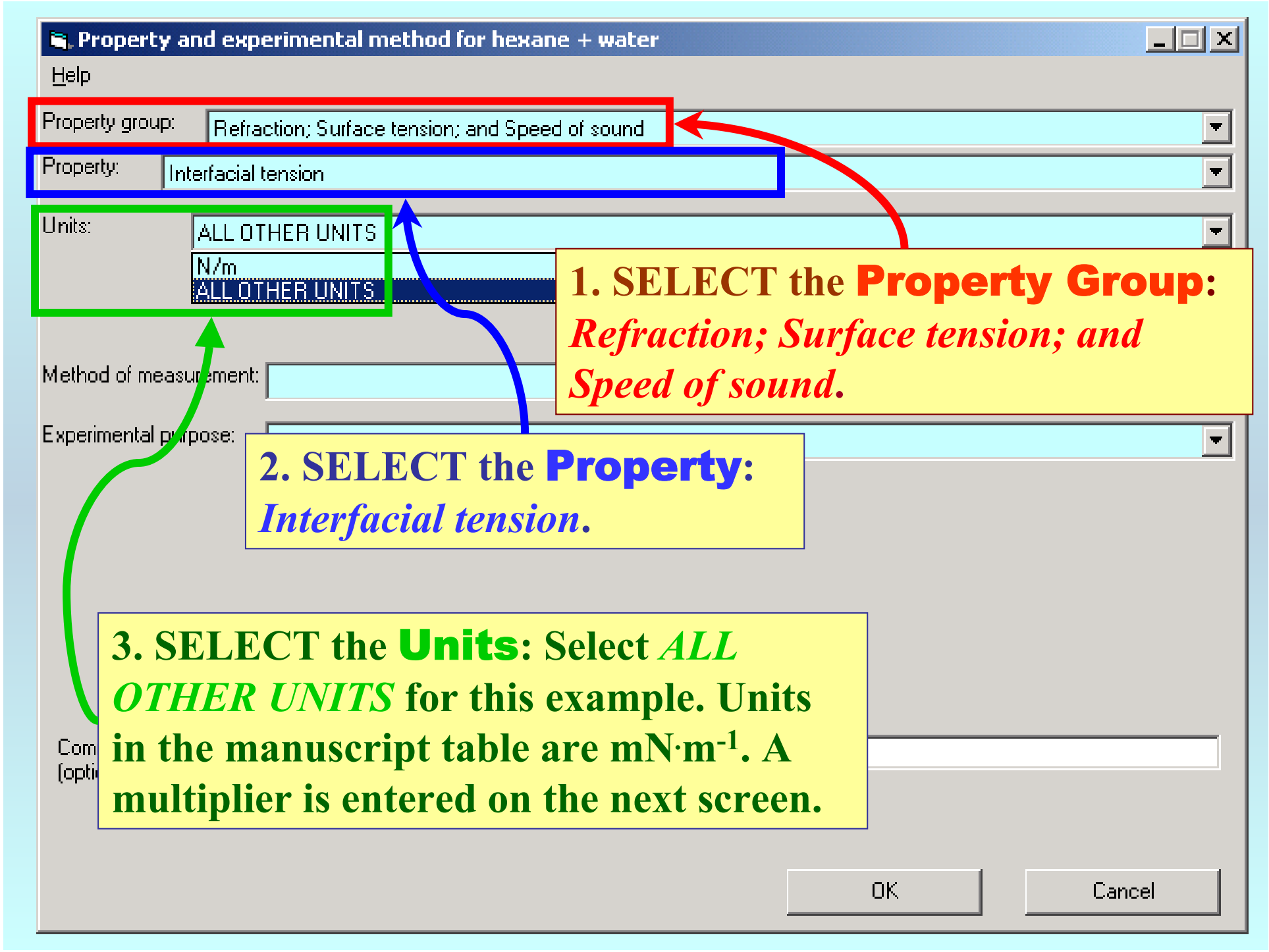
Emerging Drop Analysis

Uncertainty in interfacial tension = 0.04 $mN \cdot m^{-1}$

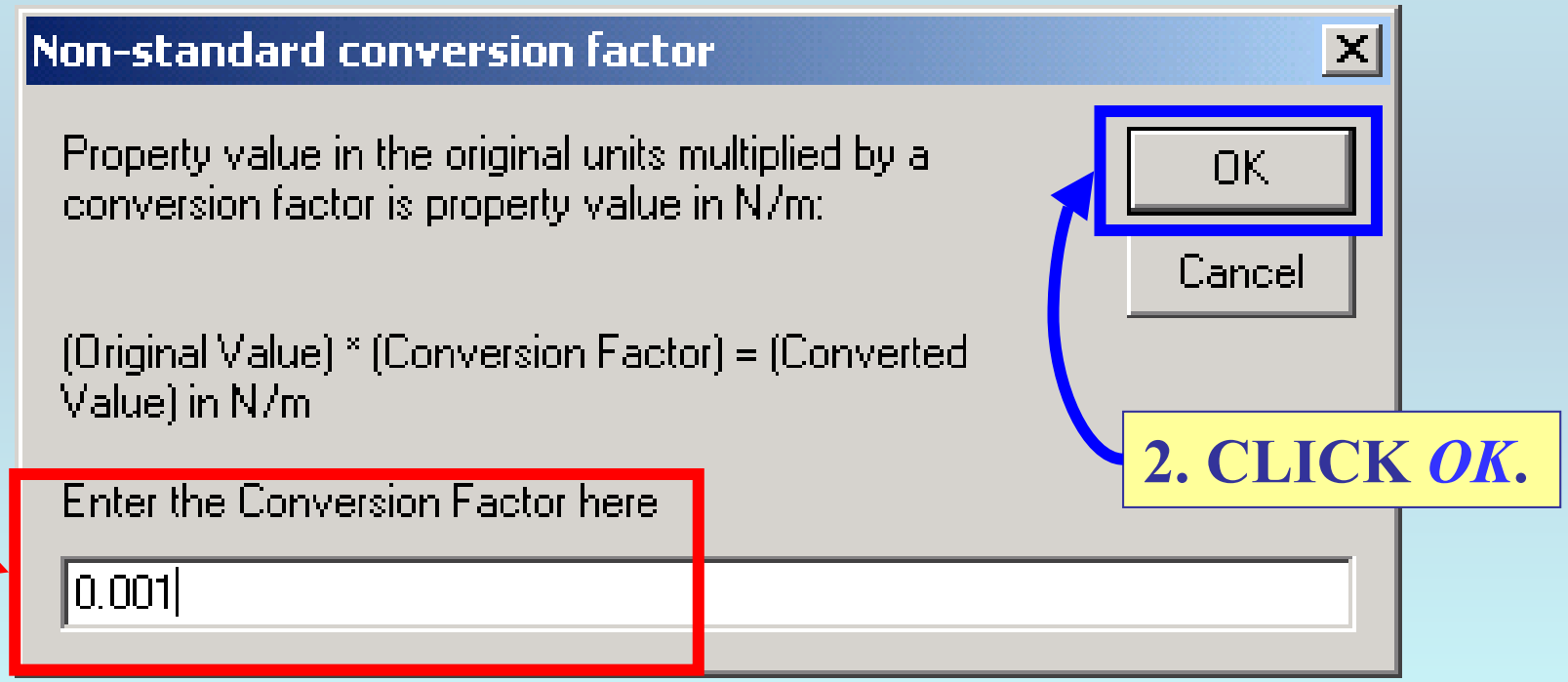
Uncertainty in temperature = 0.1 K



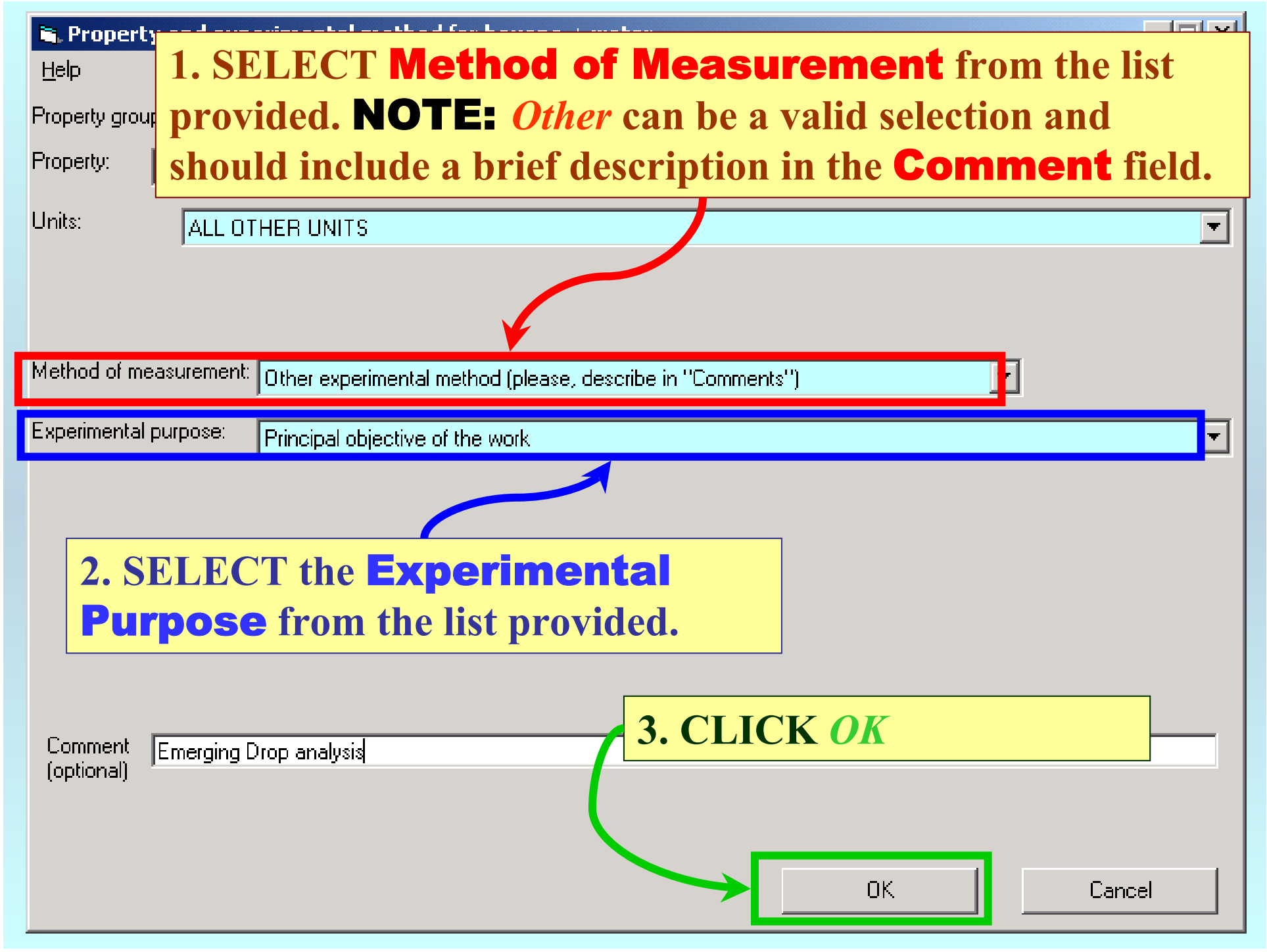
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for hexane + water
Help
Property group:
Refraction; Surface tension; and Speed of sound
Property:
Interfacial tension
Units:
ALL OTHER UNITS
N/m
ALL OTHER UNITS
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Refraction; Surface tension; and Speed of sound.
2. SELECT the Property: Interfacial tension.
3. SELECT the Units: Select ALL OTHER UNITS for this example. Units in the manuscript table are mN·m-1. A multiplier is entered on the next screen.
OK
Cancel

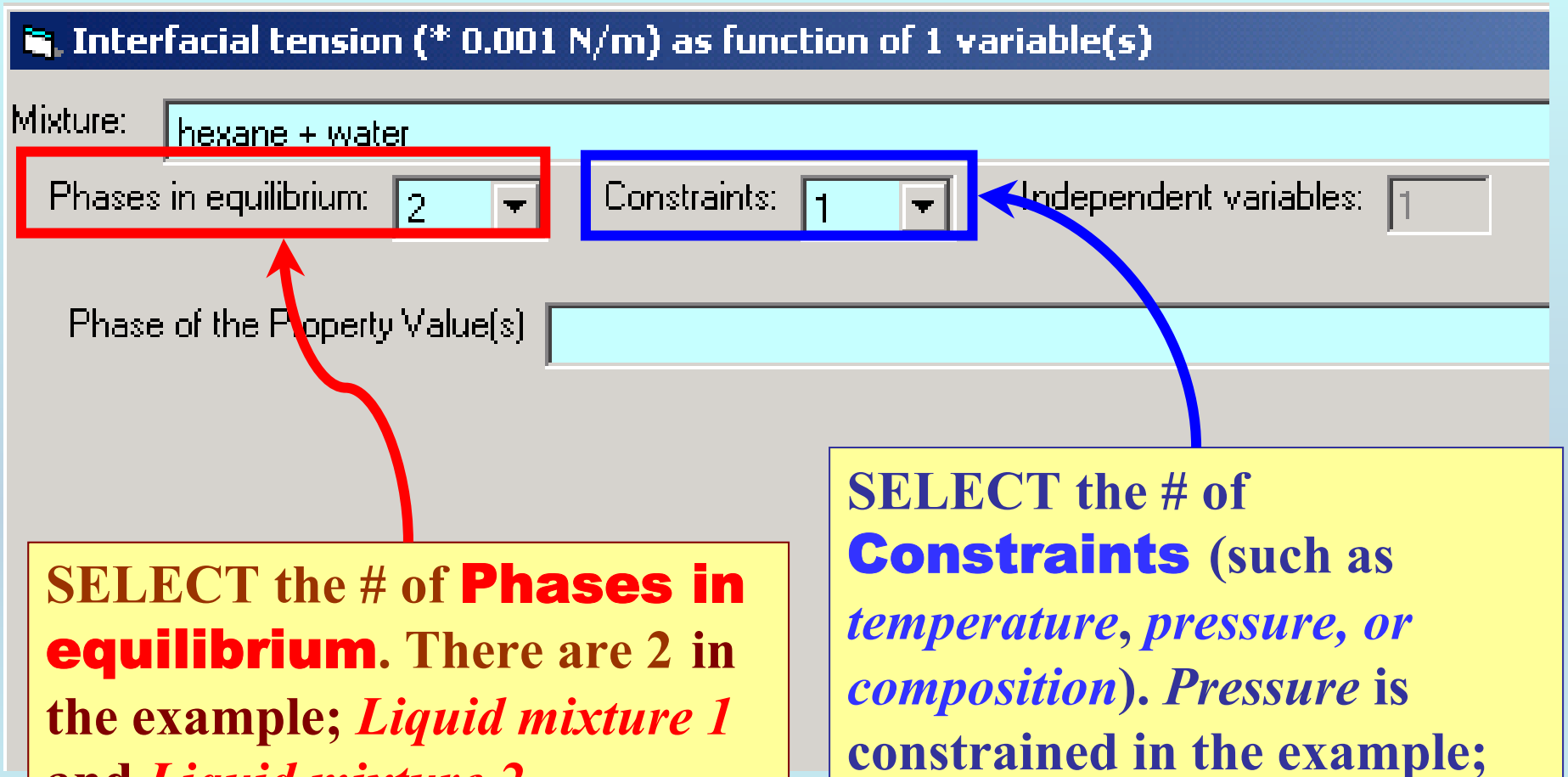
1. TYPE the required conversion factor (*0.001* for the example).



2. CLICK *OK*.

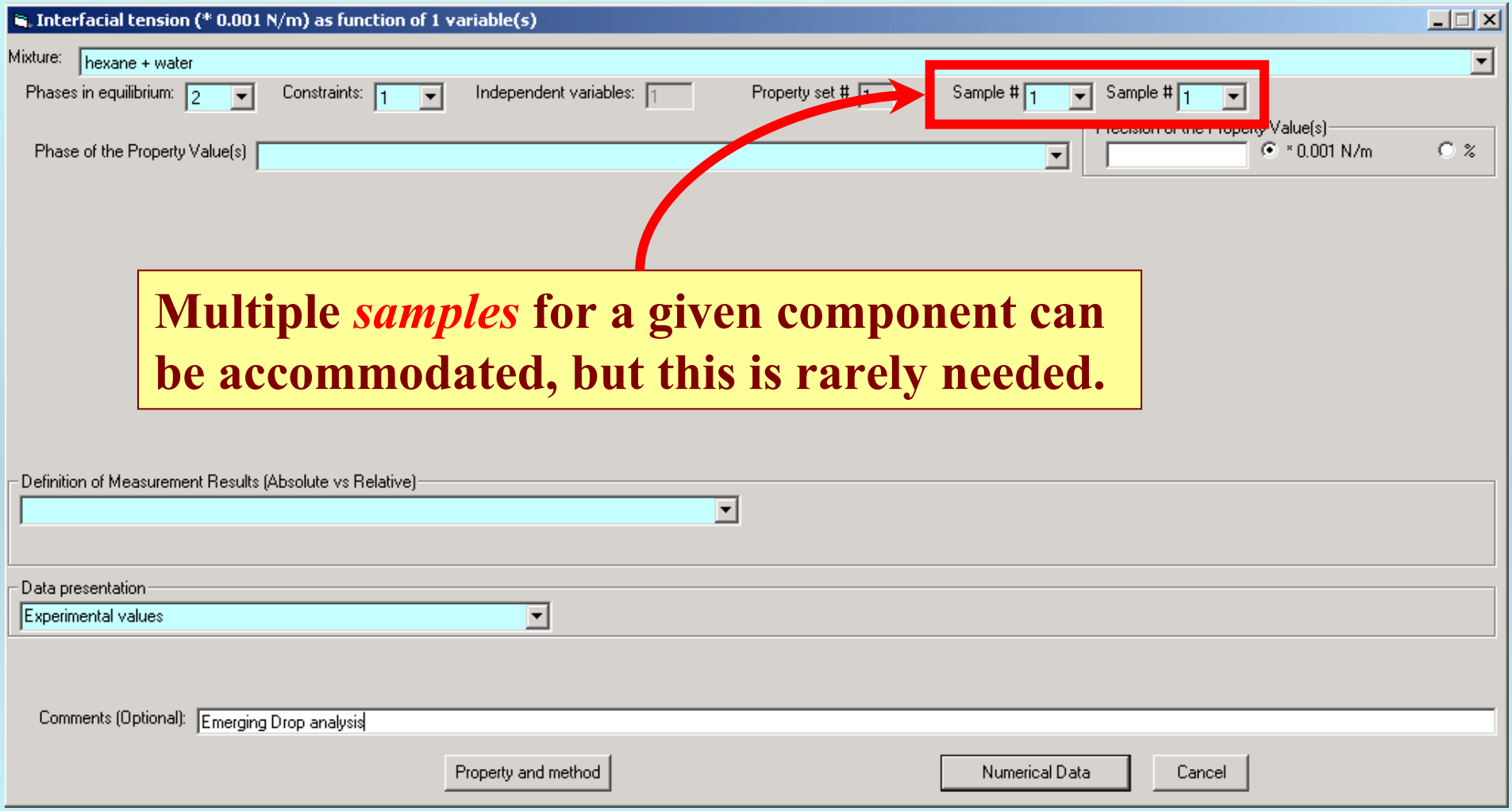

Property
Help
Property group
Property:
Units:
ALL OTHER UNITS
1. SELECT Method of Measurement from the list provided. NOTE: Other can be a valid selection and should include a brief description in the Comment field.
Method of measurement:
Other experimental method (please, describe in "Comments")
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
Emerging Drop analysis
3. CLICK OK
OK
Cancel

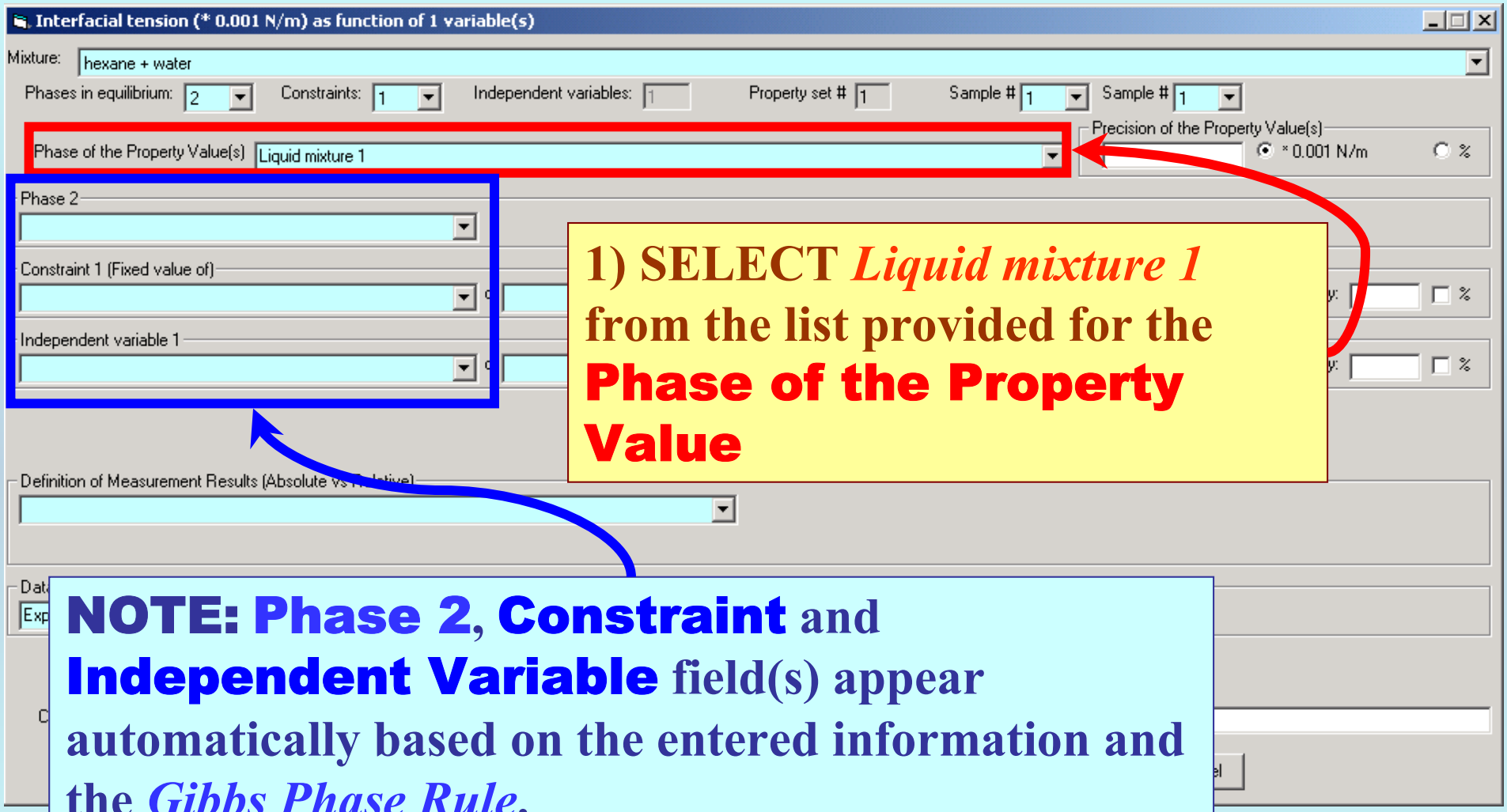
SELECTION of # of Phases in Equilibrium and # of Constraints



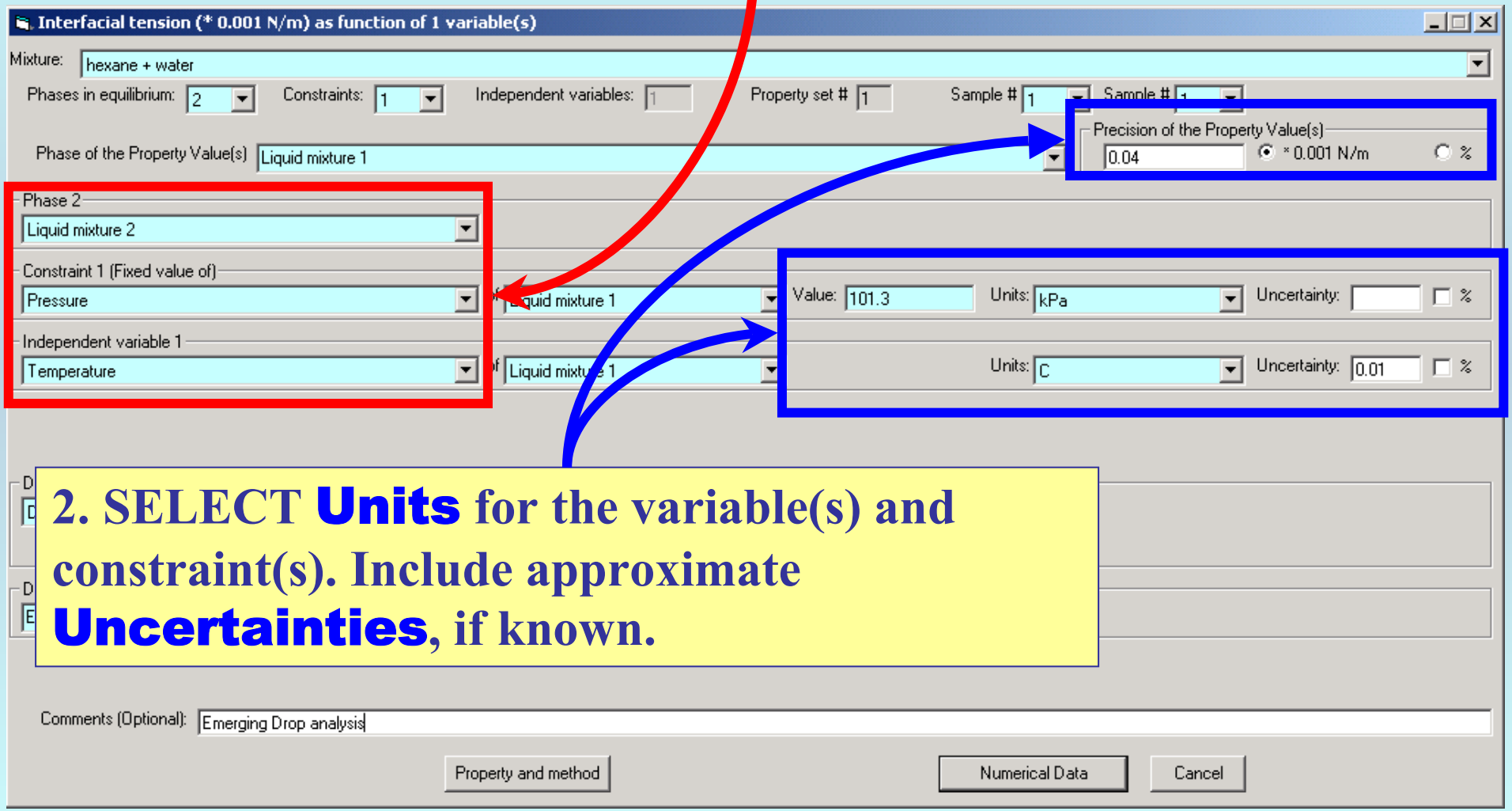
SELECT the # of **Phases in equilibrium**. There are 2 in the example; *Liquid mixture 1* and *Liquid mixture 2*.

SELECT the # of **Constraints** (such as *temperature*, *pressure, or composition*). *Pressure* is constrained in the example; p = 101.3 kPa.

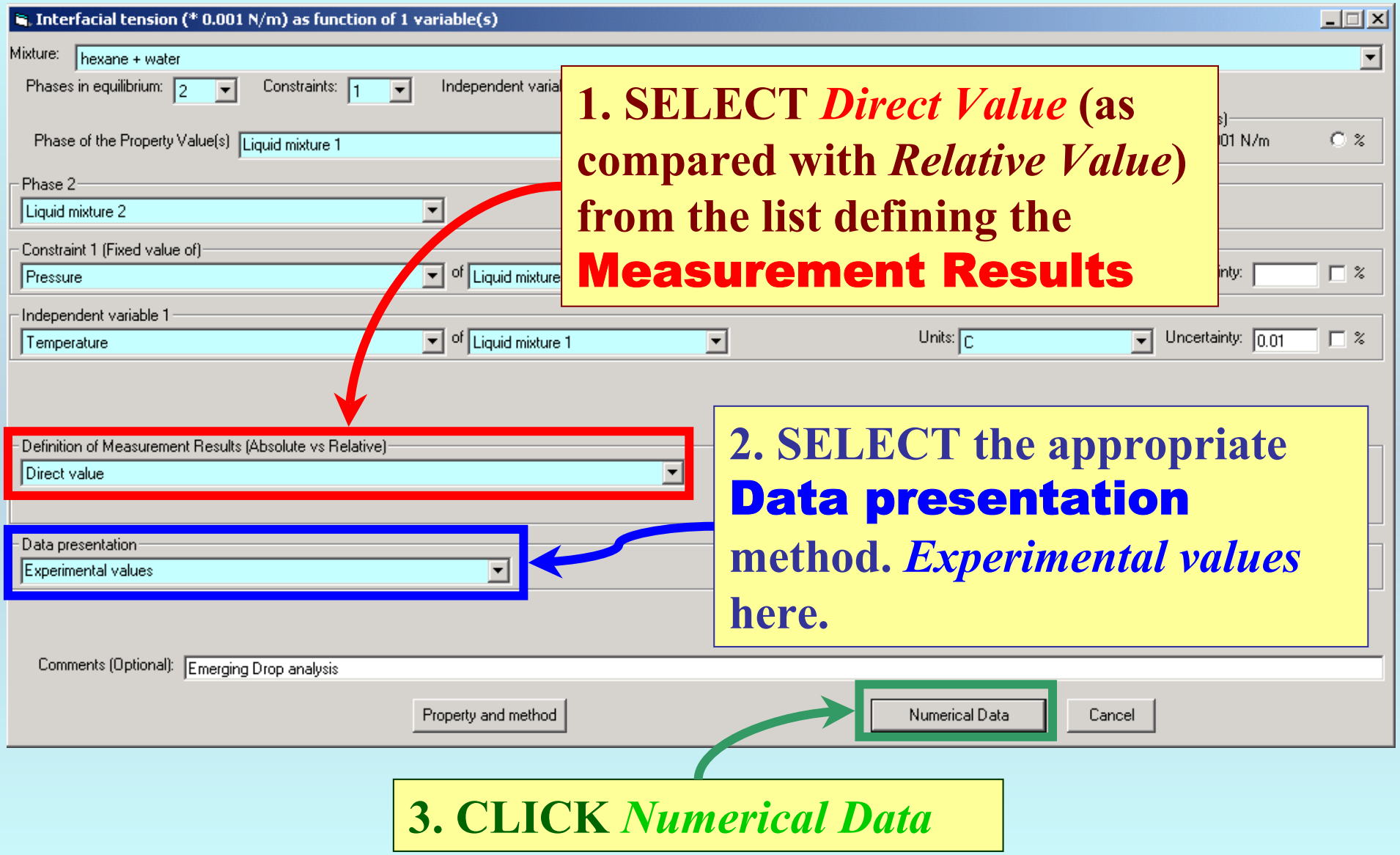

Interfacial tension (* 0.001 N/m) as function of 1 variable(s)
Mixture:
hexane + water
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
* 0.001 N/m
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Emerging Drop analysis
Property and method
Numerical Data
Cancel

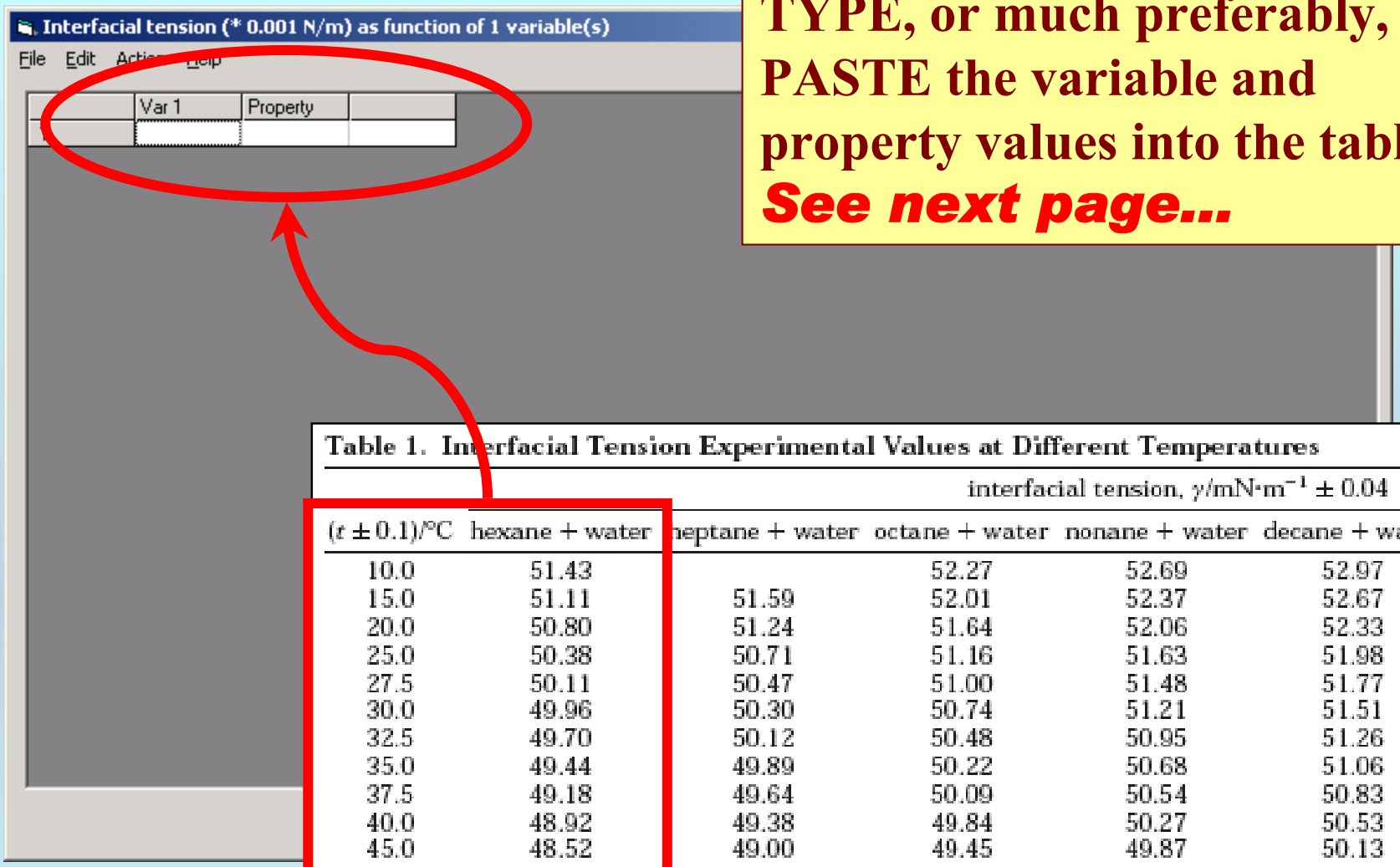

Interfacial tension (* 0.001 N/m) as function of 1 variable(s)
Mixture:
hexane + water
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid mixture 1
Precision of the Property Value(s)
* 0.001 N/m
%
Phase 2
Constraint 1 (Fixed value of)
Independent variable 1
Definition of Measurement Results (Absolute vs
1) SELECT Liquid mixture 1 from the list provided for the Phase of the Property Value
NOTE: Phase 2, Constraint and Independent Variable field(s) appear automatically based on the entered information and the Gibbs Phase Rule.

1. SELECT the Phase 2 (*Liquid mixture 2*), Constraint(s), and Independent variable(s) from the menus.



2. SELECT Units for the variable(s) and constraint(s). Include approximate Uncertainties, if known.


Interfacial tension (* 0.001 N/m) as function of 1 variable(s)
Mixture: hexane + water
Phases in equilibrium: 2
Constraints: 1
Phase of the Property Value(s): Liquid mixture 1
Phase 2
Liquid mixture 2
Constraint 1 (Fixed value of)
Pressure
of Liquid mixture
Independent variable 1
Temperature
of Liquid mixture 1
Units: C
Uncertainty: 0.01
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional): Emerging Drop analysis
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. Interfacial Tension Experimental Values at Different Temperatures

	interfacial tension, γ/mN·m^{-1} ± 0.04				
(t ± 0.1)/°C	hexane + water	heptane + water	octane + water	nonane + water	decane + water
10.0	51.43		52.27	52.69	52.97
15.0	51.11	51.59	52.01	52.37	52.67
20.0	50.80	51.24	51.64	52.06	52.33
25.0	50.38	50.71	51.16	51.63	51.98
27.5	50.11	50.47	51.00	51.48	51.77
30.0	49.96	50.30	50.74	51.21	51.51
32.5	49.70	50.12	50.48	50.95	51.26
35.0	49.44	49.89	50.22	50.68	51.06
37.5	49.18	49.64	50.09	50.54	50.83
40.0	48.92	49.38	49.84	50.27	50.53
45.0	48.52	49.00	49.45	49.87	50.13
50.0	48.13	48.55	48.95	49.36	49.78
55.0			48.58	49.09	49.45
60.0			48.32	48.82	49.21

Interfacial tension (* 0.001 N/m) as function of 1 variable(s)

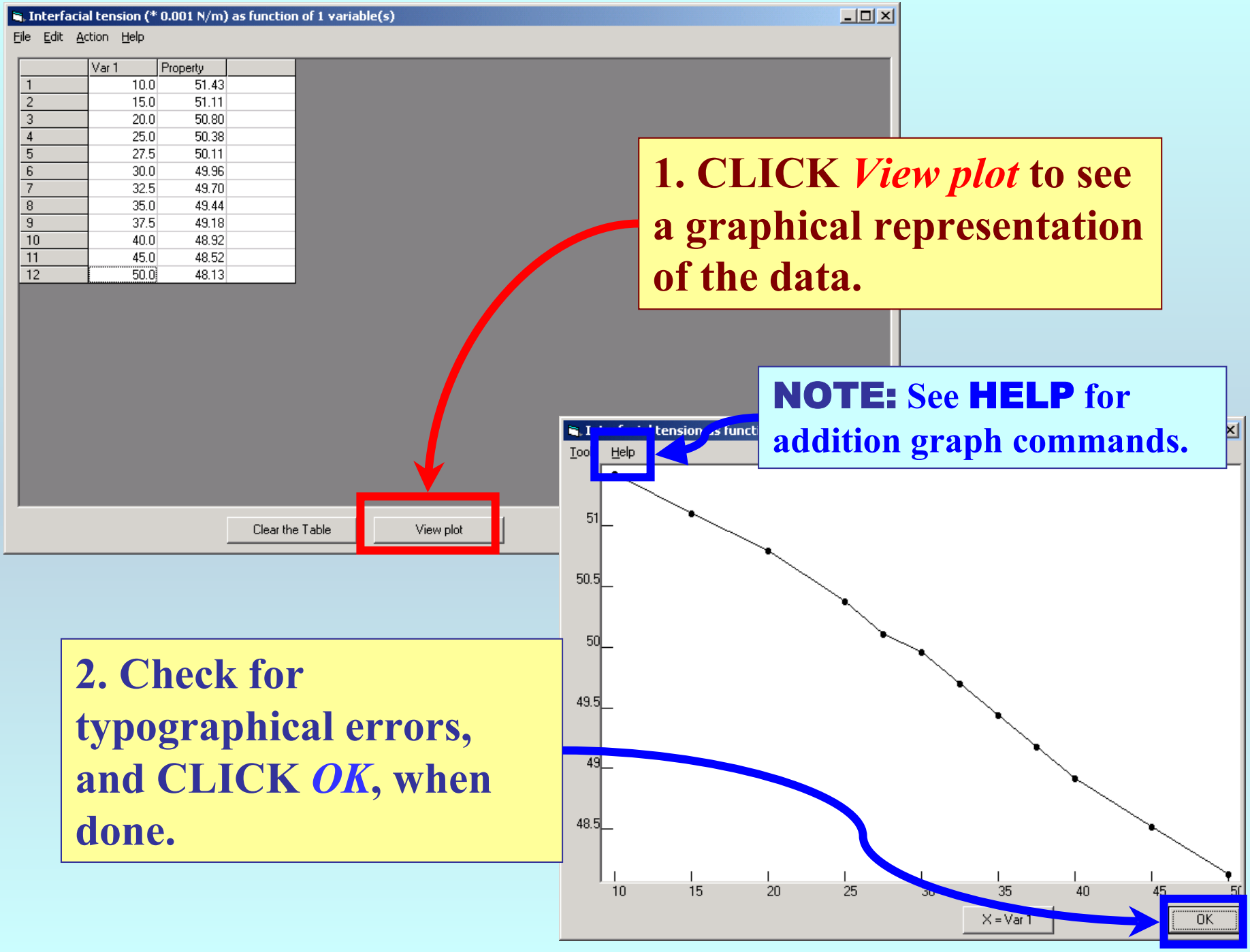
File Edit Action Help

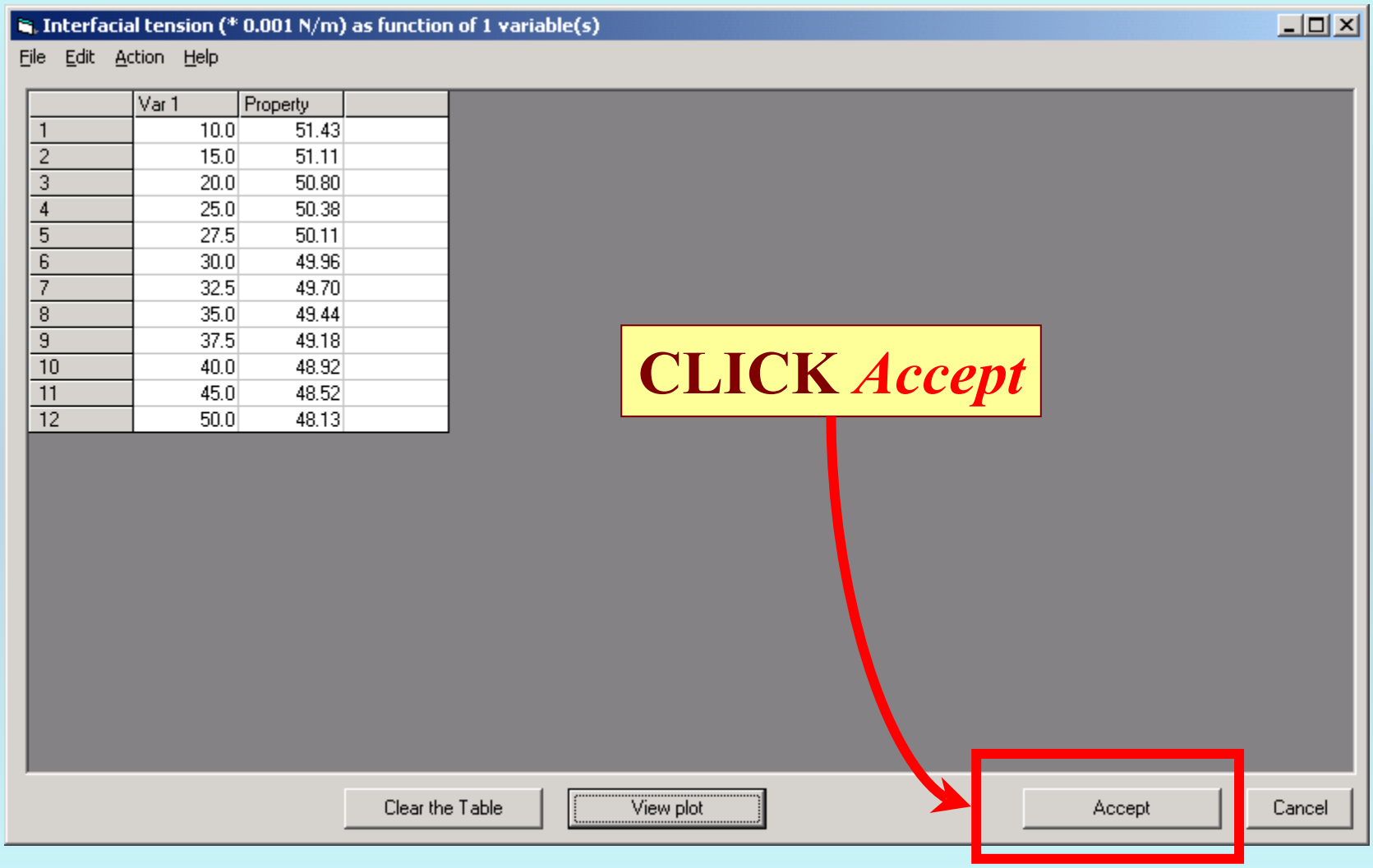
	Var 1	Property
1	10.0	51.43
2	15.0	51.11
3	20.0	50.80
4	25.0	50.38
5	27.5	50.11
6	30.0	49.96
7	32.5	49.70
8	35.0	49.44
9	37.5	49.18
10	40.0	48.92
11	45.0	48.52
12	50.0	48.13

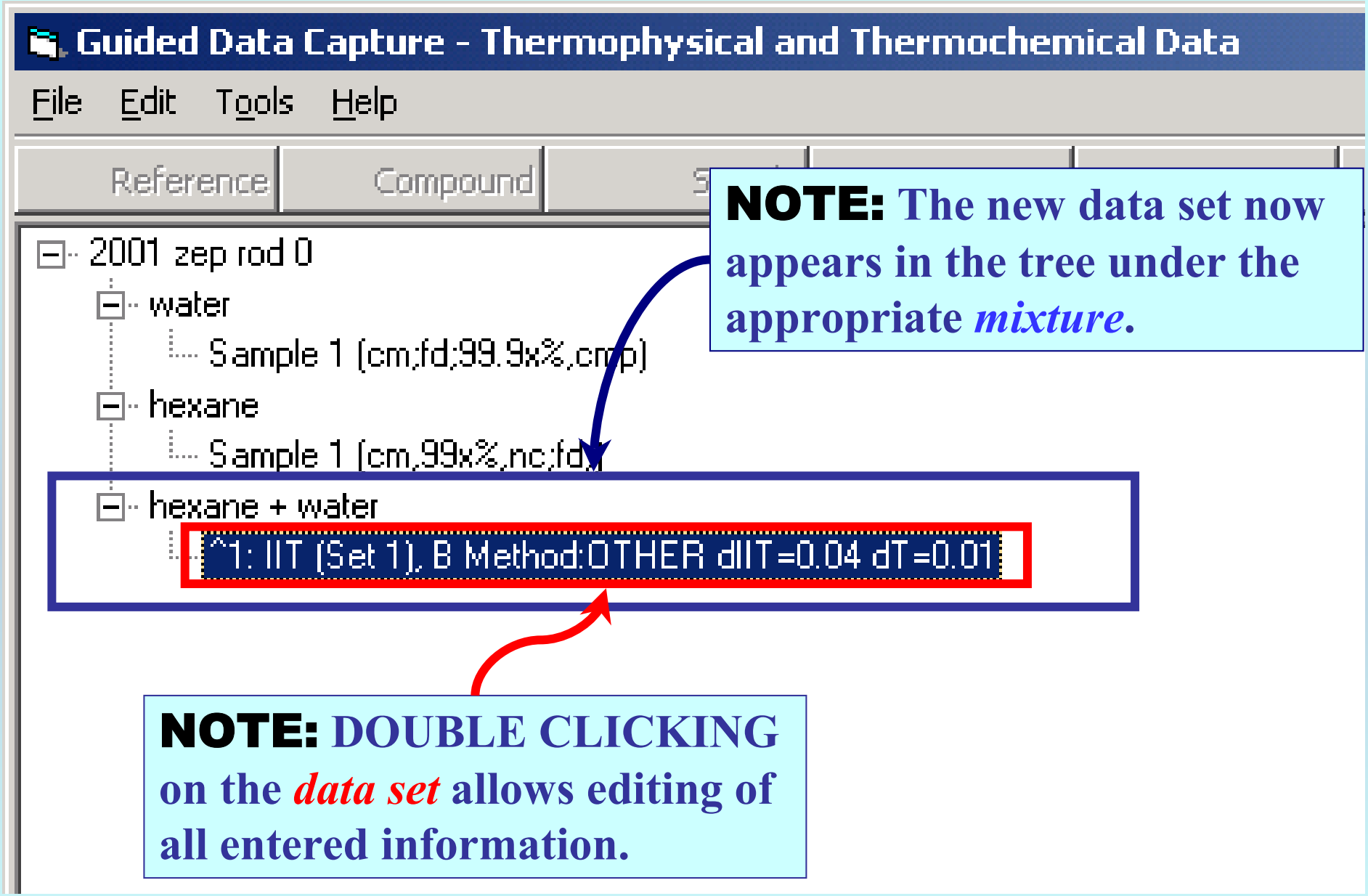
Table 1. Interfacial Tension Experimental Values at Different Temperatures

	interfacial tension, γ/mN·m^{-1} ± 0.04				
(t ± 0.1)/°C	hexane + water	heptane + water	octane + water	nonane + water	decane + water
10.0	51.43		52.27	52.69	52.97
15.0	51.11	51.59	52.01	52.37	52.67
20.0	50.80	51.24	51.64	52.06	52.33
25.0	50.38	50.71	51.16	51.63	51.98
27.5	50.11	50.47	51.00	51.48	51.77
30.0	49.96	50.30	50.74	51.21	51.51
32.5	49.70	50.12	50.48	50.95	51.26
35.0	49.44	49.89	50.22	50.68	51.06
37.5	49.18	49.64	50.09	50.54	50.83
40.0	48.92	49.38	49.84	50.27	50.53
45.0	48.52	49.00	49.45	49.87	50.13
50.0	48.13	48.55	48.95	49.36	49.78
55.0			48.58	49.09	49.45
60.0			48.32	48.82	49.21

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.)


Interfacial tension (* 0.001 N/m) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 10.0 51.43
2 15.0 51.11
3 20.0 50.80
4 25.0 50.38
5 27.5 50.11
6 30.0 49.96
7 32.5 49.70
8 35.0 49.44
9 37.5 49.18
10 40.0 48.92
11 45.0 48.52
12 50.0 48.13
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
NOTE: See HELP for addition graph commands.
Too Help
51
50.5
50
49.5
49
48.5
10 15 20 25 35 40 45
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.


Interfacial tension (* 0.001 N/m) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 10.0 51.43
2 15.0 51.11
3 20.0 50.80
4 25.0 50.38
5 27.5 50.11
6 30.0 49.96
7 32.5 49.70
8 35.0 49.44
9 37.5 49.18
10 40.0 48.92
11 45.0 48.52
12 50.0 48.13
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference
Compound
2001 zep rod 0
water
Sample 1 [cm;fd;99.9x%,cmp]
hexane
Sample 1 [cm,99x%,nc;fd]
hexane + water
^1: IIT (Set 1), B Method:OTHER dIIT=0.04 dT=0.01
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, if all properties have been captured.**