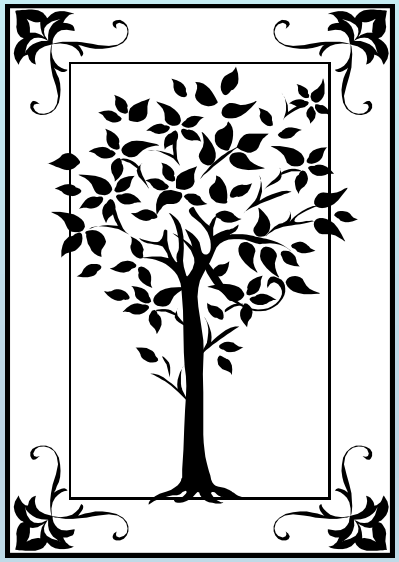
METADATA AND NUMERICAL DATA CAPTURE: DENSITY (2 component mixture)

Guided Data Capture (GDC)



This tutorial decribes
METADATA AND NUMERICAL DATA CAPTURE:
for **DENSITIES (2 components)**
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 2002, *47*, 811−815

Density and Refractive Index at 298.15 K and Vapor−Liquid Equilibria at 101.3 kPa for Four Binary Systems of Methanol, *n*-Propanol, *n*-Butanol, or Isobutanol with *N*-Methylpiperazine

Shuda Chen,† Qunfang Lei, and Wenjun Fang*

Department of Chemistry, Zhejiang University, Hangzhou 310027, Zhejiang, People's Republic of China

Density and refractive index data at 298.15 K, and isobaric vapor−liquid equilibrium (VLE) measurements at 101.3 kPa were reported for four binary systems of methanol, *n*-propanol, *n*-butanol, or isobutanol with *N*-methylpiperazine. Excess molar volumes and refractive index deviations were calculated. The measurement results exhibit no azeotropes for VLE, negative values for excess molar volume, and positive deviations from ideality for the refractive index over the whole mole fraction range. Liquid-phase activity coefficients and vapor-phase fugacity coefficients were estimated taking into account the nonideal nature of the vapor and liquid phases. The VLE data were shown to be thermodynamically consistent and were correlated by the UNIQUAC liquid-phase activity coefficient model with temperature-dependent parameters.

Densities (liquid phase) for (methanol + N-methylpiperazine) at T = 298.15 K and p = 101.3 kPa

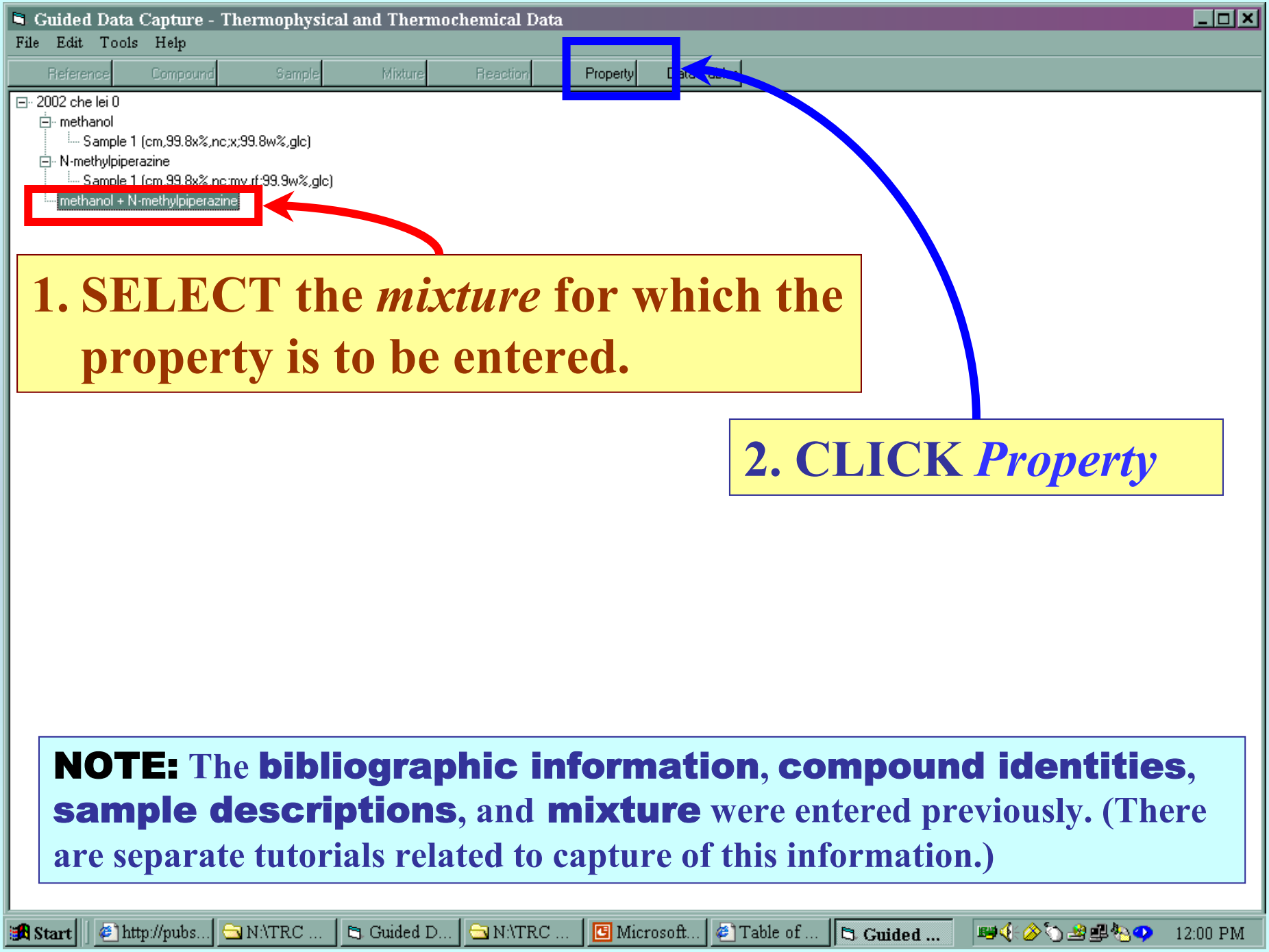
Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + *N*-Methylpiperazine (2) at 298.15 K

x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
Methanol (1) + NMP (2)			*n*-Propanol (1) + NMP (2)		
0.0498	0.899 54	−0.225	0.0483	0.898 02	−0.187
0.1050	0.899 14	−0.463	0.1012	0.895 74	−0.361
0.1491	0.898 68	−0.641	0.1395	0.894 07	−0.492
0.2052	0.897 88	−0.848	0.1465	0.893 78	−0.519
0.2503	0.897 23	−1.020	0.1950	0.891 38	−0.661
0.2996	0.896 17	−1.178	0.2439	0.888 98	−0.815
0.3488	0.894 96	−1.330	0.2936	0.886 06	−0.930
0.3989	0.893 39	−1.465	0.3473	0.882 79	−1.056
0.4492	0.891 59	−1.593	0.3914	0.879 95	−1.153
0.5006	0.889 11	−1.686	0.4476	0.875 98	−1.255
0.5618	0.885 69	−1.787	0.4913	0.872 65	−1.323
0.6001	0.882 75	−1.807	0.5452	0.868 03	−1.370
0.6497	0.878 42	−1.822	0.5934	0.863 55	−1.395
0.7052	0.872 25	−1.789	0.6424	0.858 59	−1.399
0.7521	0.865 54	−1.707	0.6922	0.853 04	−1.372
0.8001	0.856 87	−1.563	0.7420	0.846 78	−1.299
0.8490	0.845 58	−1.340	0.7941	0.839 47	−1.177
0.8978	0.831 09	−1.023	0.8425	0.831 79	−1.006
0.9490	0.811 44	−0.571	0.8954	0.822 30	−0.749
			0.9474	0.811 76	−0.419

The data set considered here.

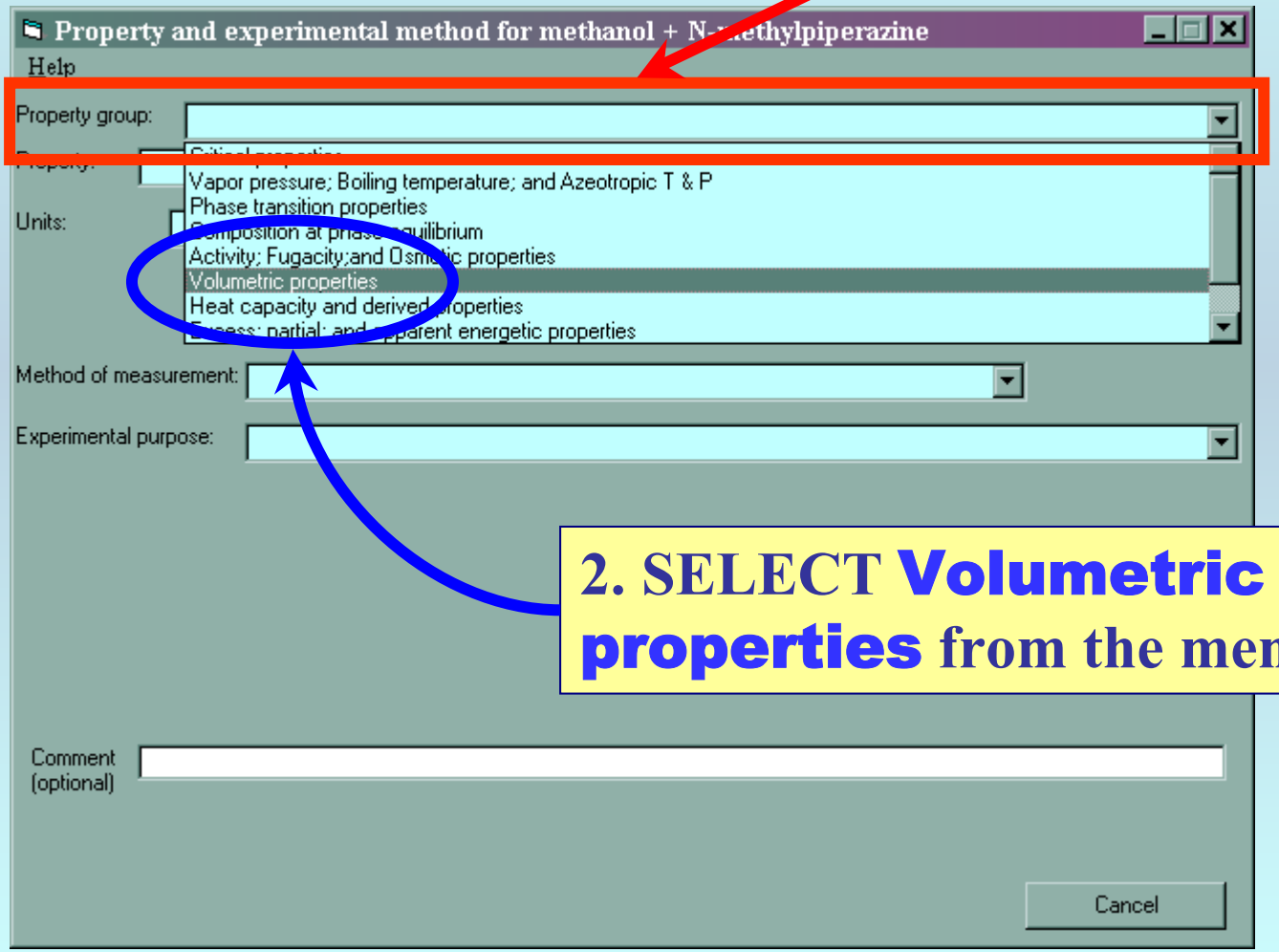
Experimental Method:

Densities of all the samples were measured by using a vibrating tube digital densimeter, model DMA 602 (Anton Paar), thermostated with a circulating-water bath with a precision of ±0.01 K. Refractive indices were determined


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property
2002 che lei 0
methanol
Sample 1 (cm,99.8x%,nc;x;99.8w%,glc)
N-methylpiperazine
Sample 1 (cm,99.8x%,nc;my,rf;99.9w%,glc)
methanol + N-methylpiperazine
1. SELECT the mixture for which the property is to be entered.
2. CLICK Property
NOTE: The bibliographic information, compound identities, sample descriptions, and mixture were entered previously. (There are separate tutorials related to capture of this information.)
Start
http://pubs...
N:\TRC ...
Guided D...
N:\TRC ...
Microsoft...
Table of ...
Guided ...
12:00 PM

Property Group selection

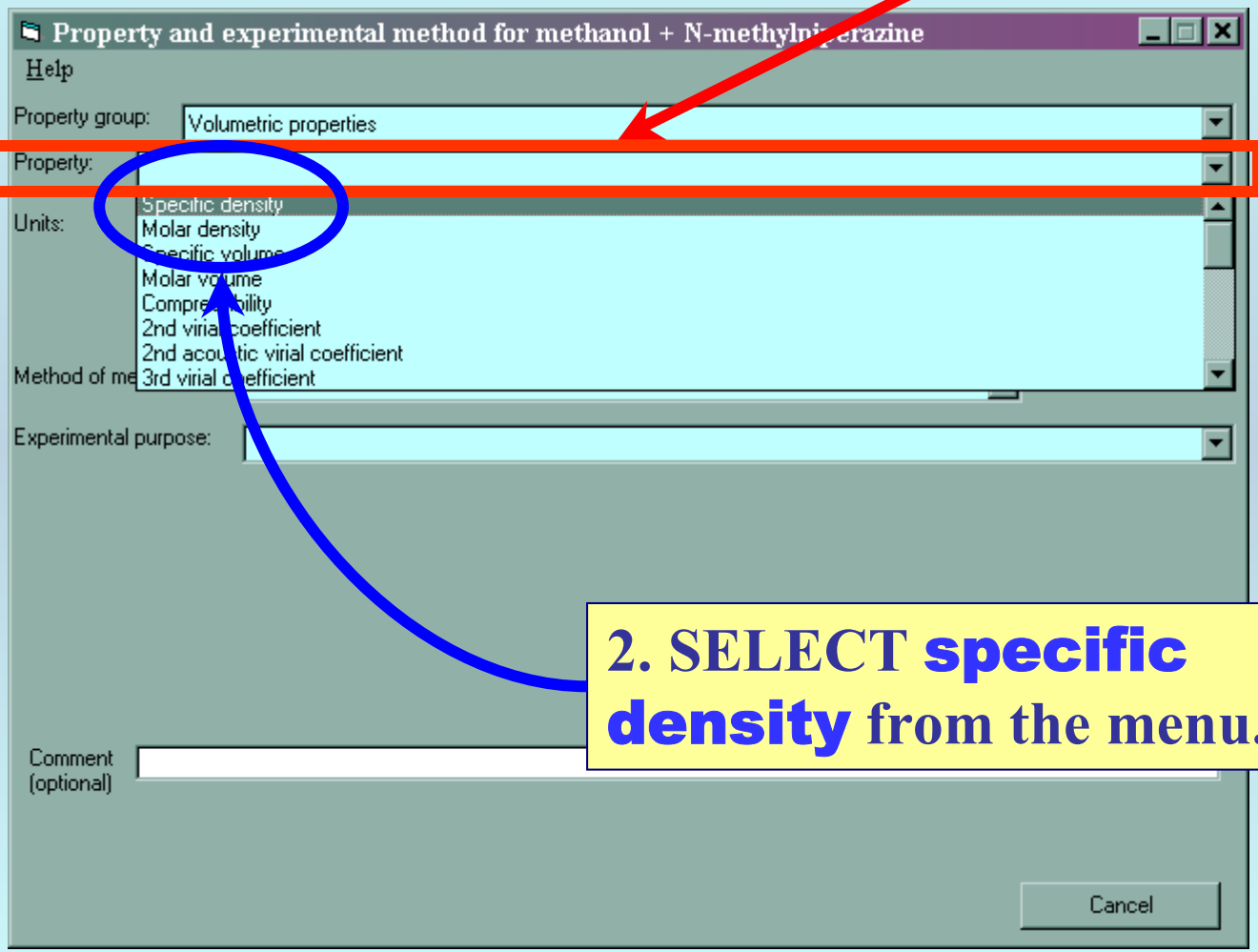
1. CLICK in the **property group** field.



2. SELECT **Volumetric properties** from the menu.

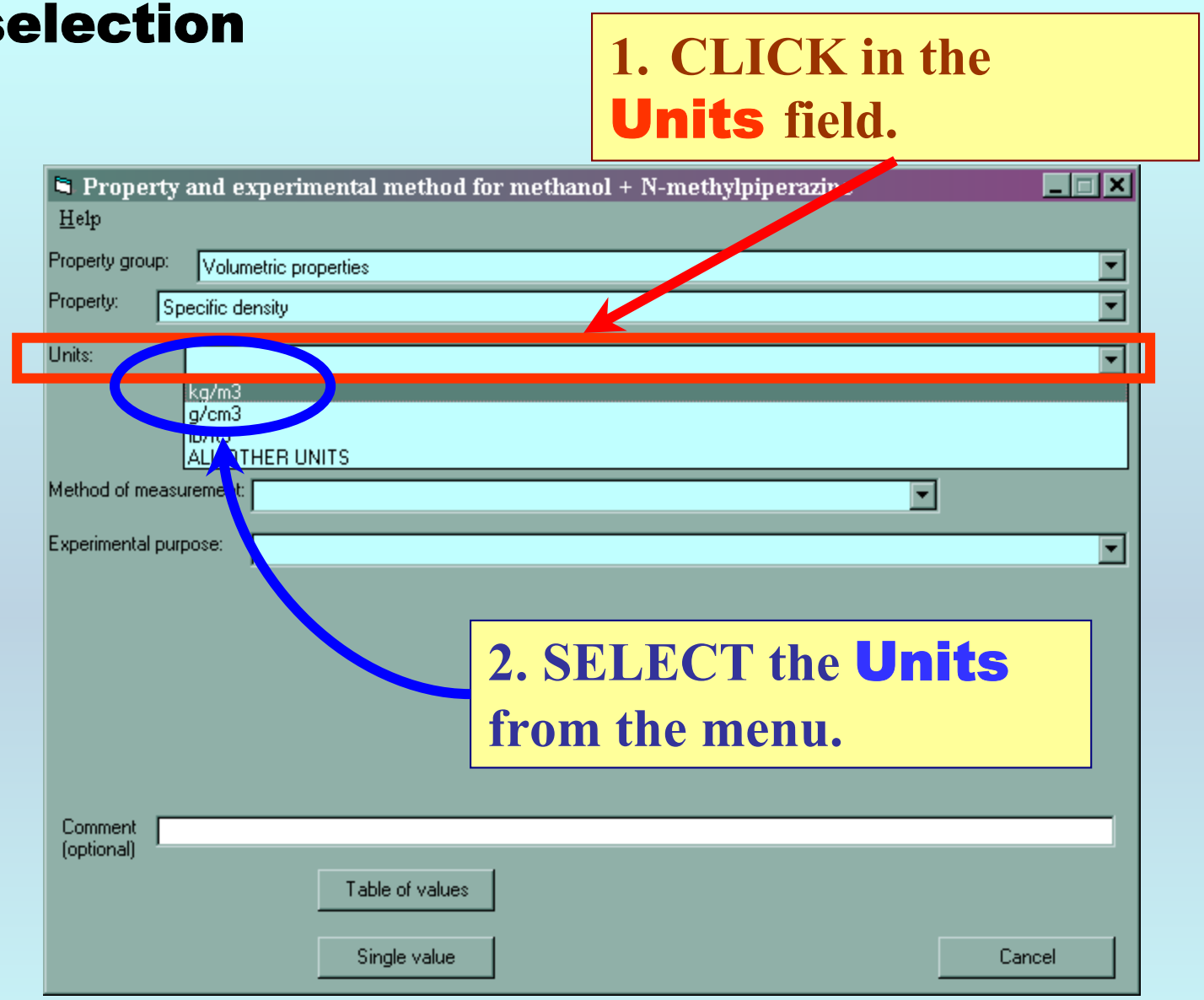
Property selection

1. CLICK in the **Property** field.



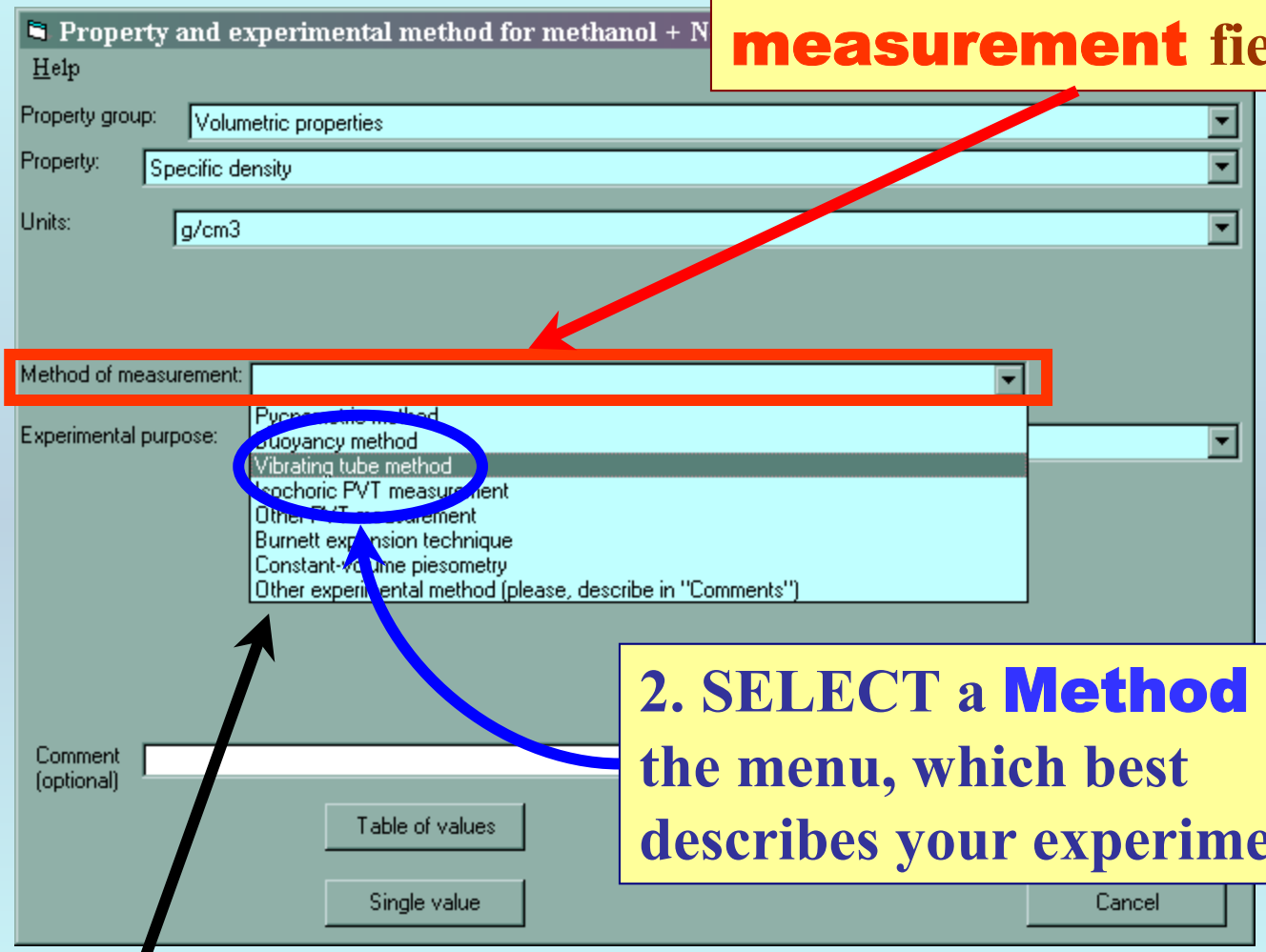
2. SELECT **specific density** from the menu.

Units selection



Method selection

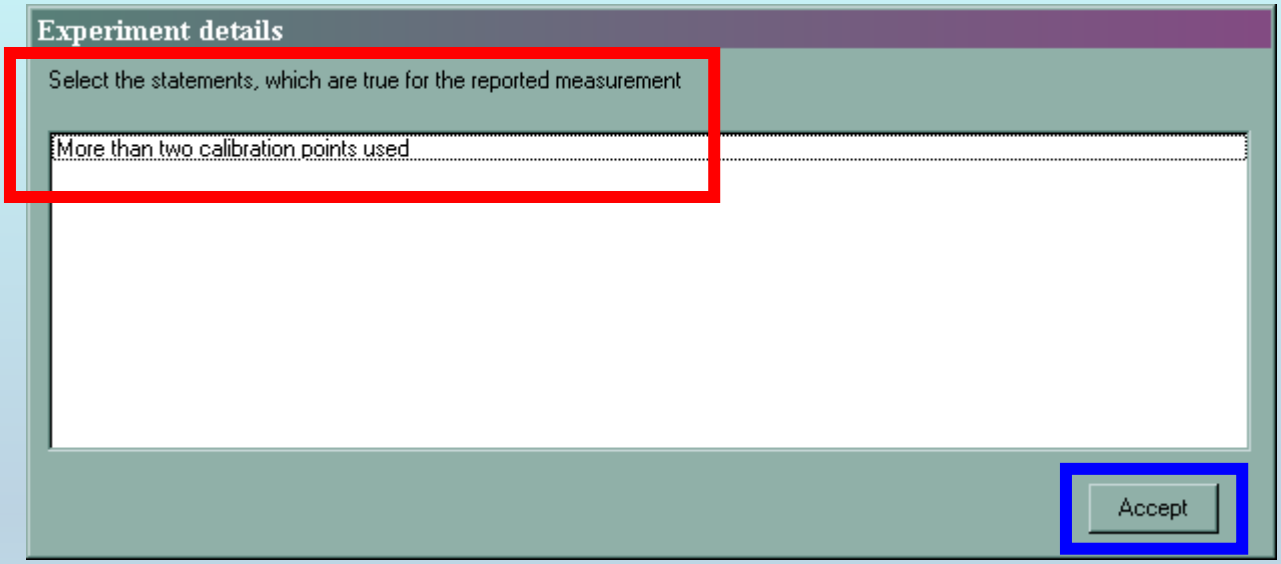
1. CLICK in the **Method of measurement** field.



2. SELECT a **Method** from the menu, which best describes your experiment

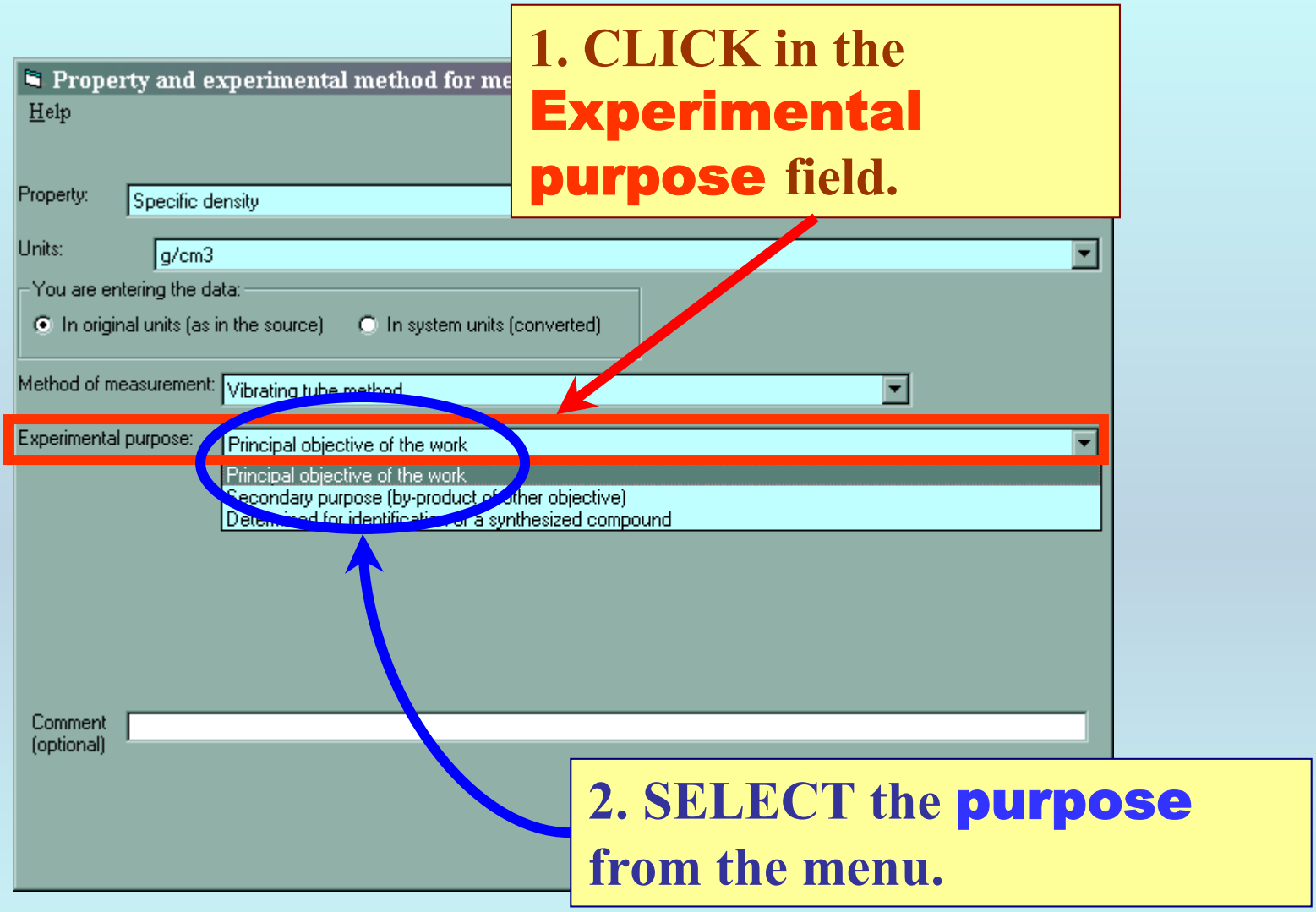
Note: ***Other*** **is an option. A one sentence description or a reference is often adequate.**

Method detail selection

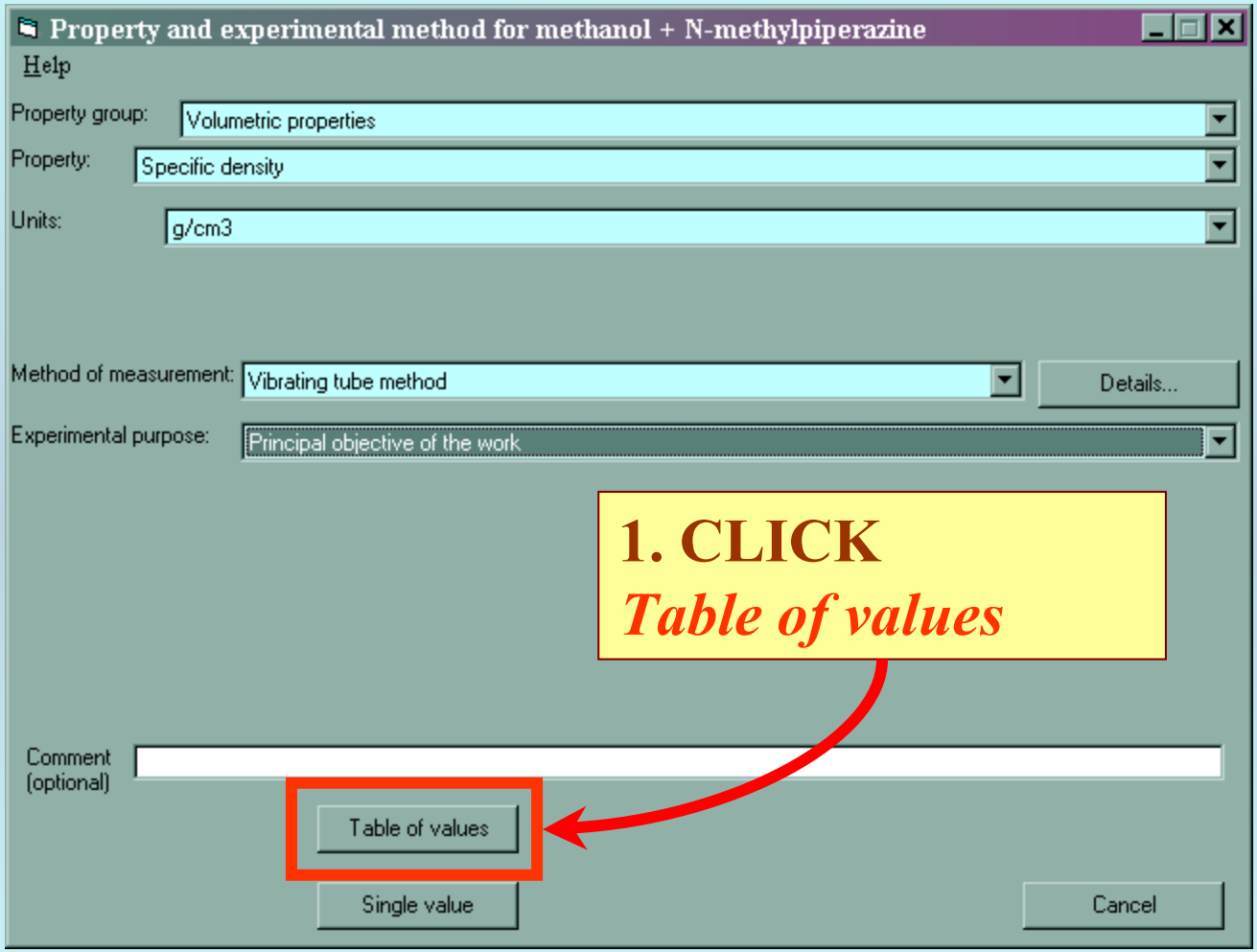


Note: For a few methods, additional details are requested. SELECT those statements that apply, and CLICK *Accept*.

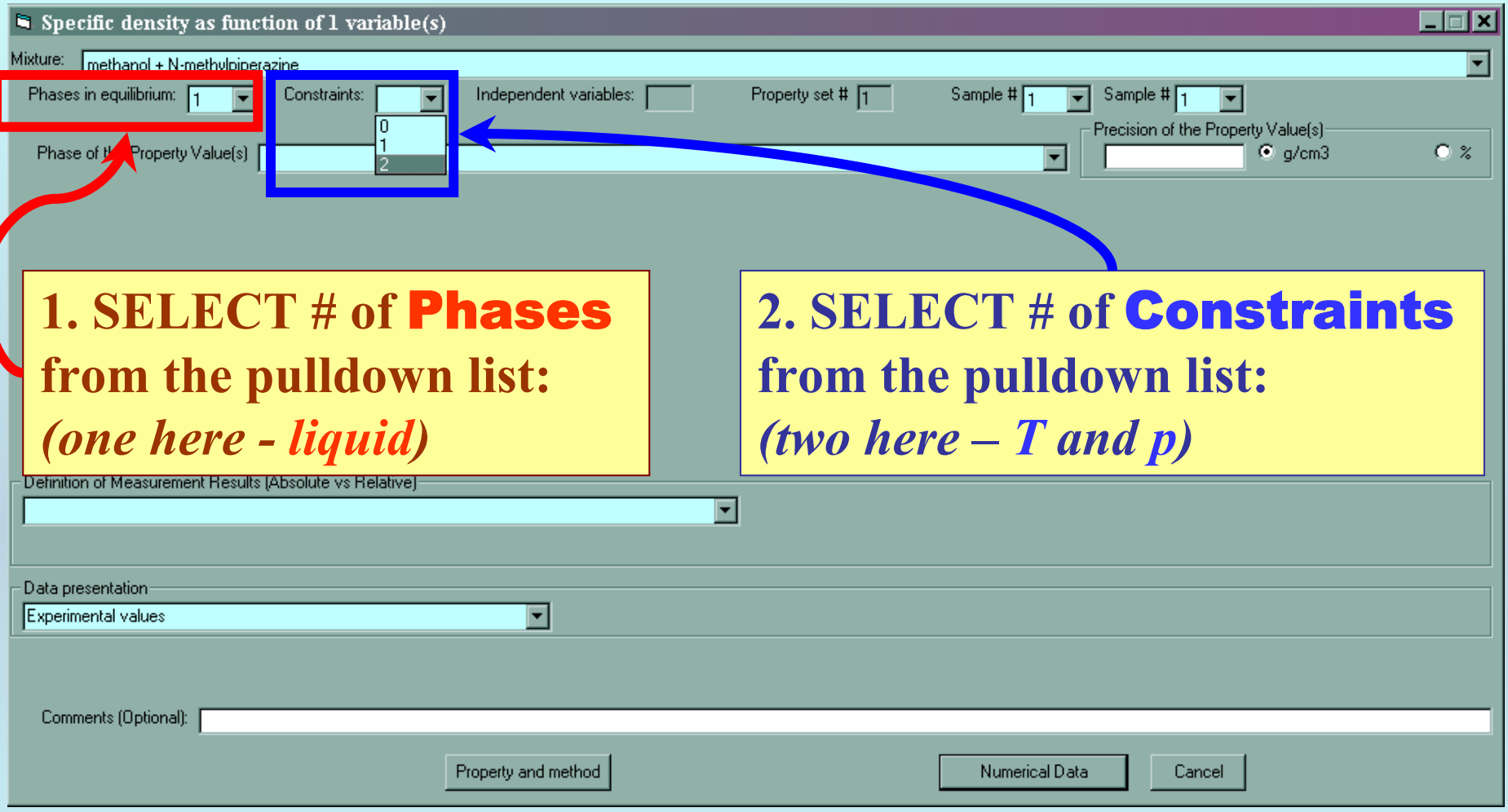
Experimental purpose selection

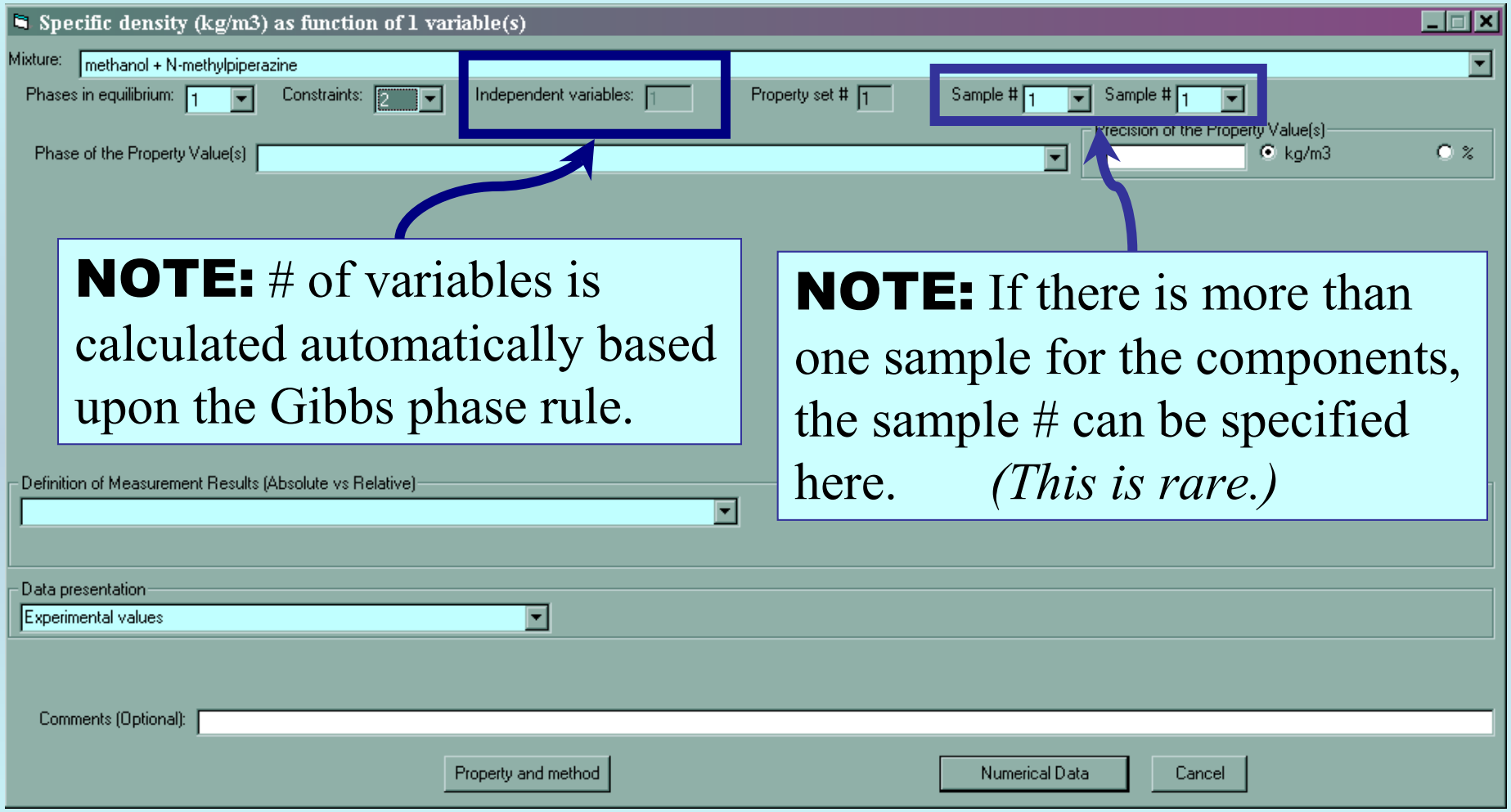


Form is complete...

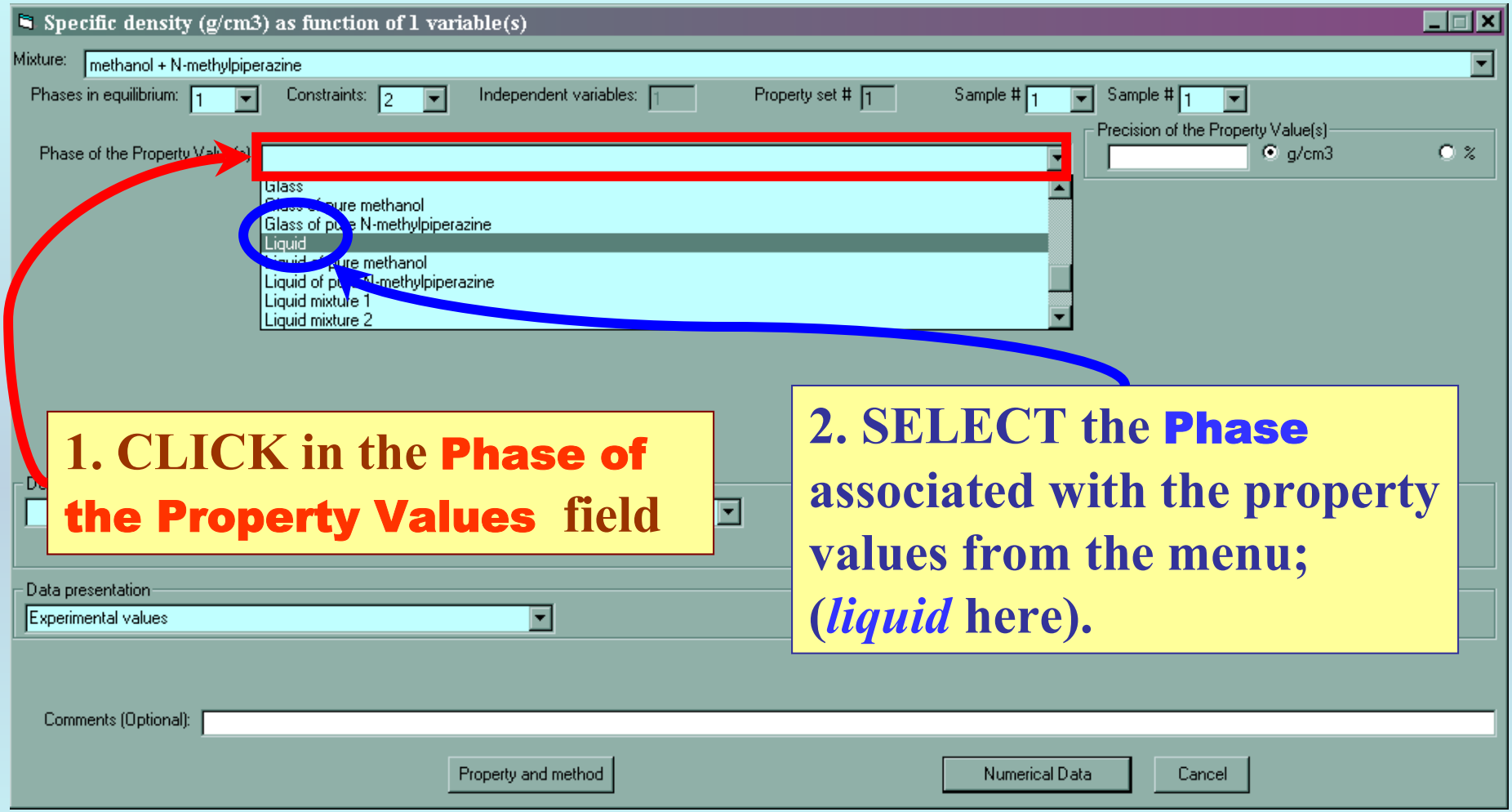


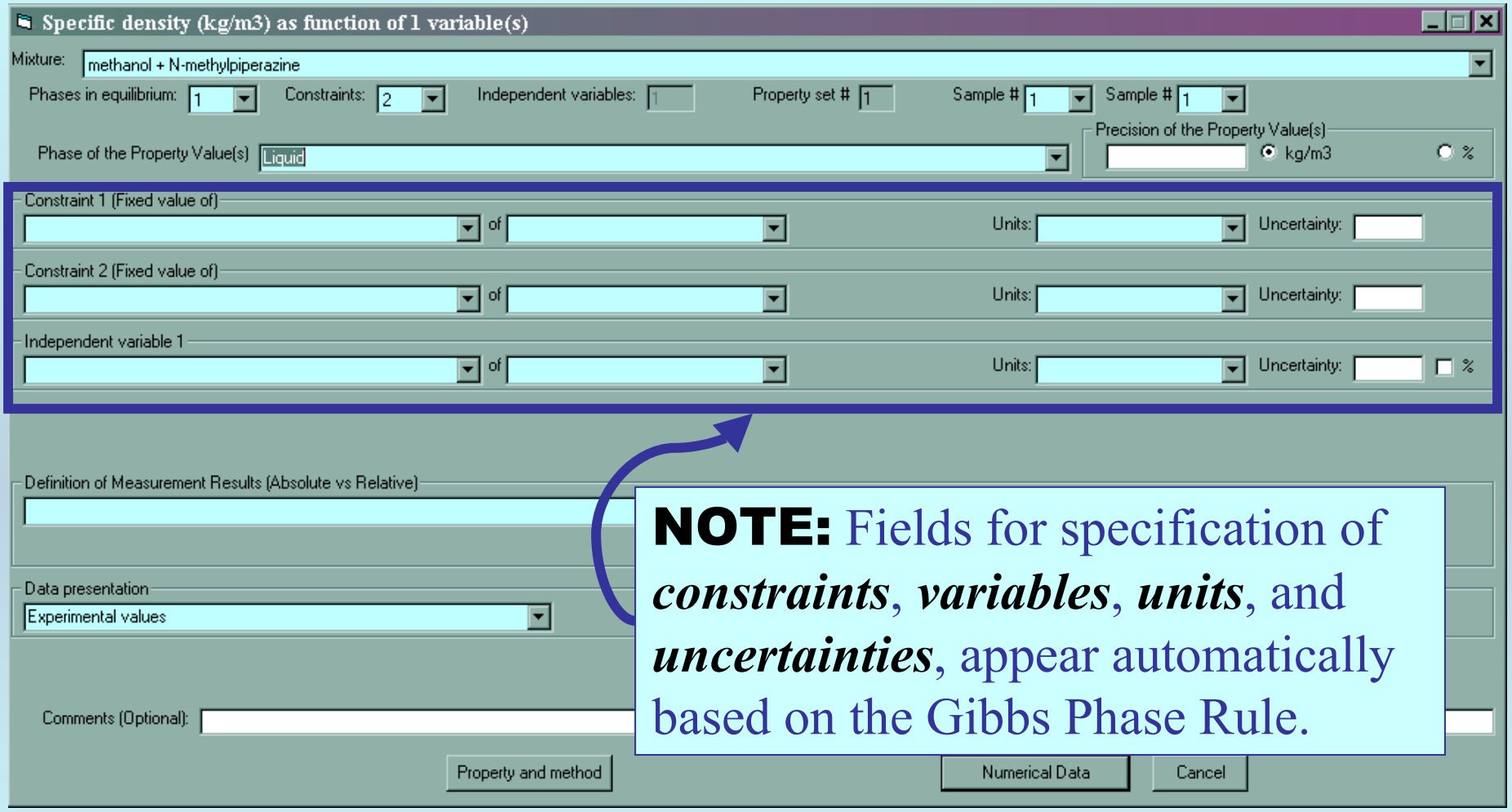
Specification of phases and constraints




Specific density (kg/m3) as function of 1 variable(s)
Mixture:
methanol + N-methylpiperazine
Phases in equilibrium:
1
Constraints:
2
Independent variables:
1
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
kg/m3
%
NOTE: # of variables is calculated automatically based upon the Gibbs phase rule.
NOTE: If there is more than one sample for the components, the sample # can be specified here. (This is rare.)
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel

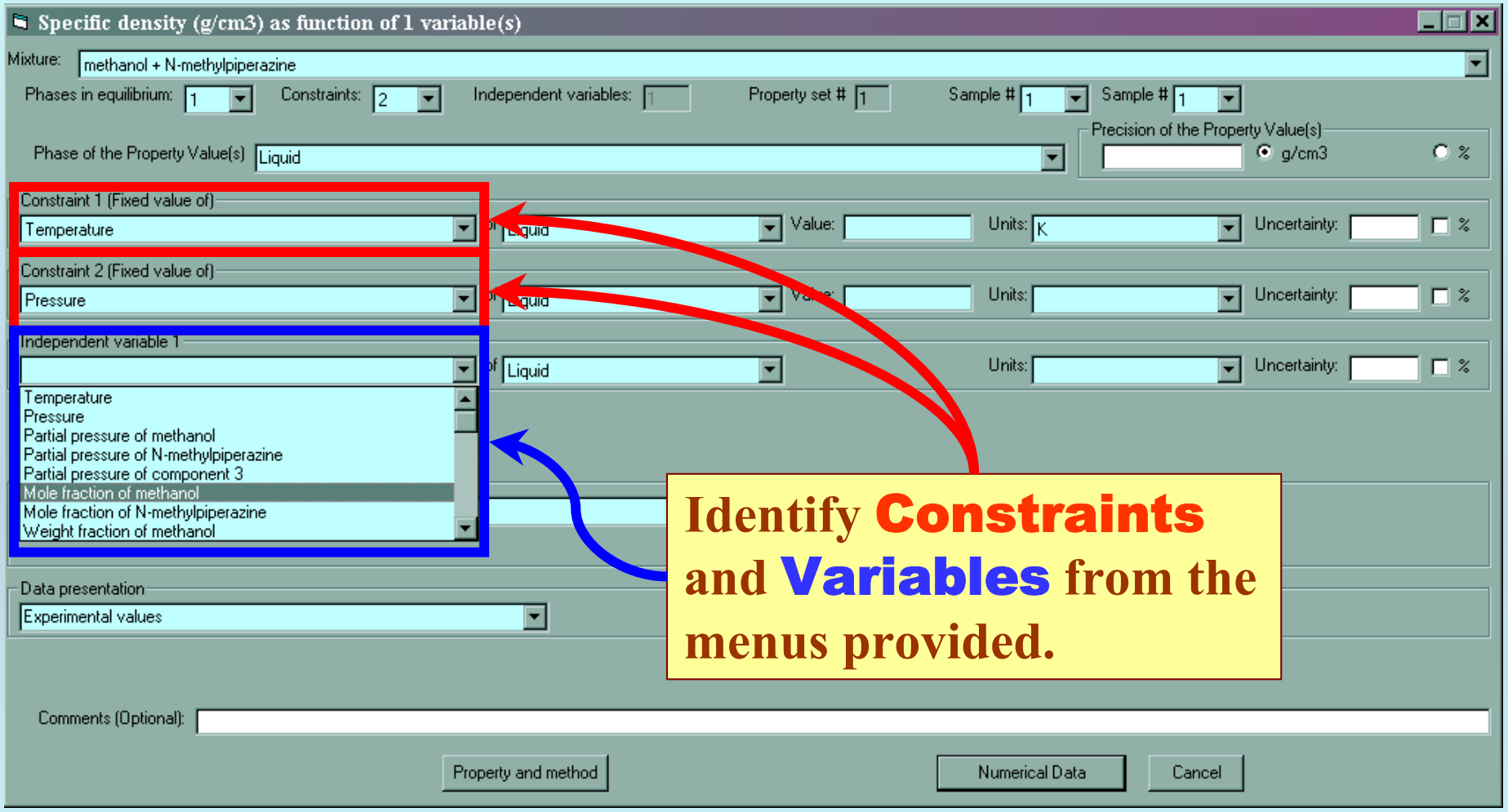
Phase of the property value selection



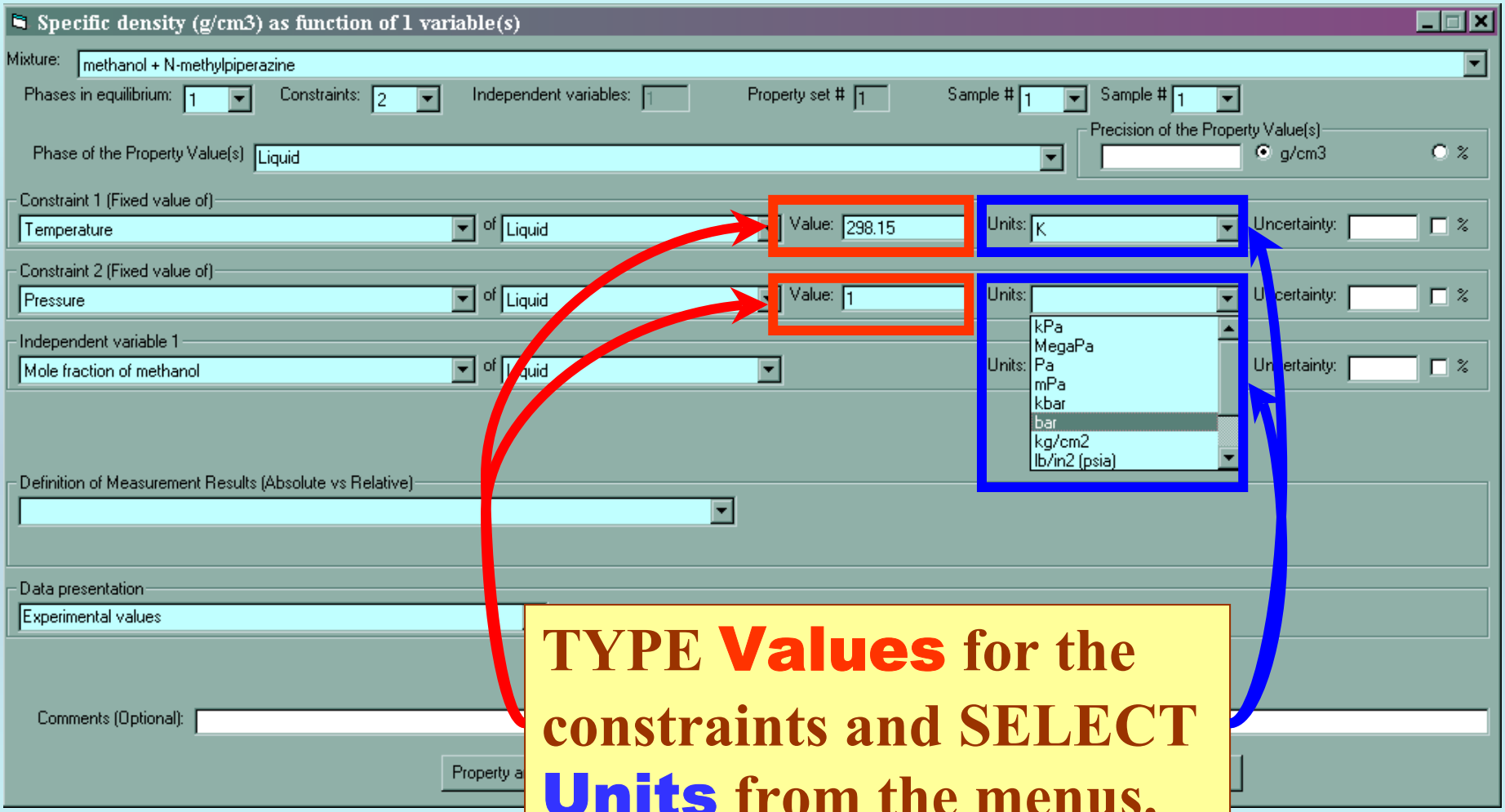


NOTE: Fields for specification of ***constraints***, ***variables***, ***units***, and ***uncertainties***, appear automatically based on the Gibbs Phase Rule.

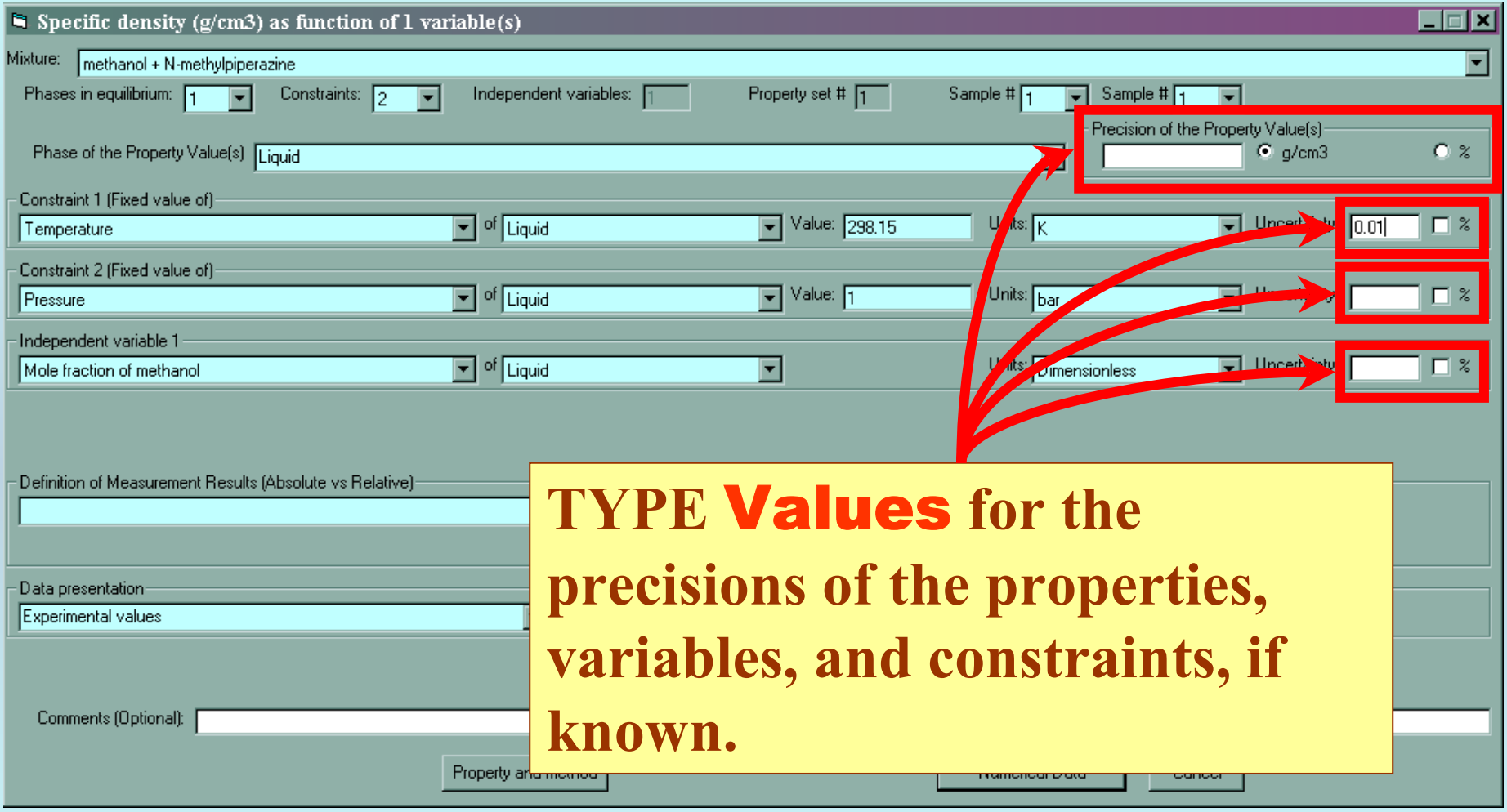
Variable and constraint identification



Entry of values for constraints

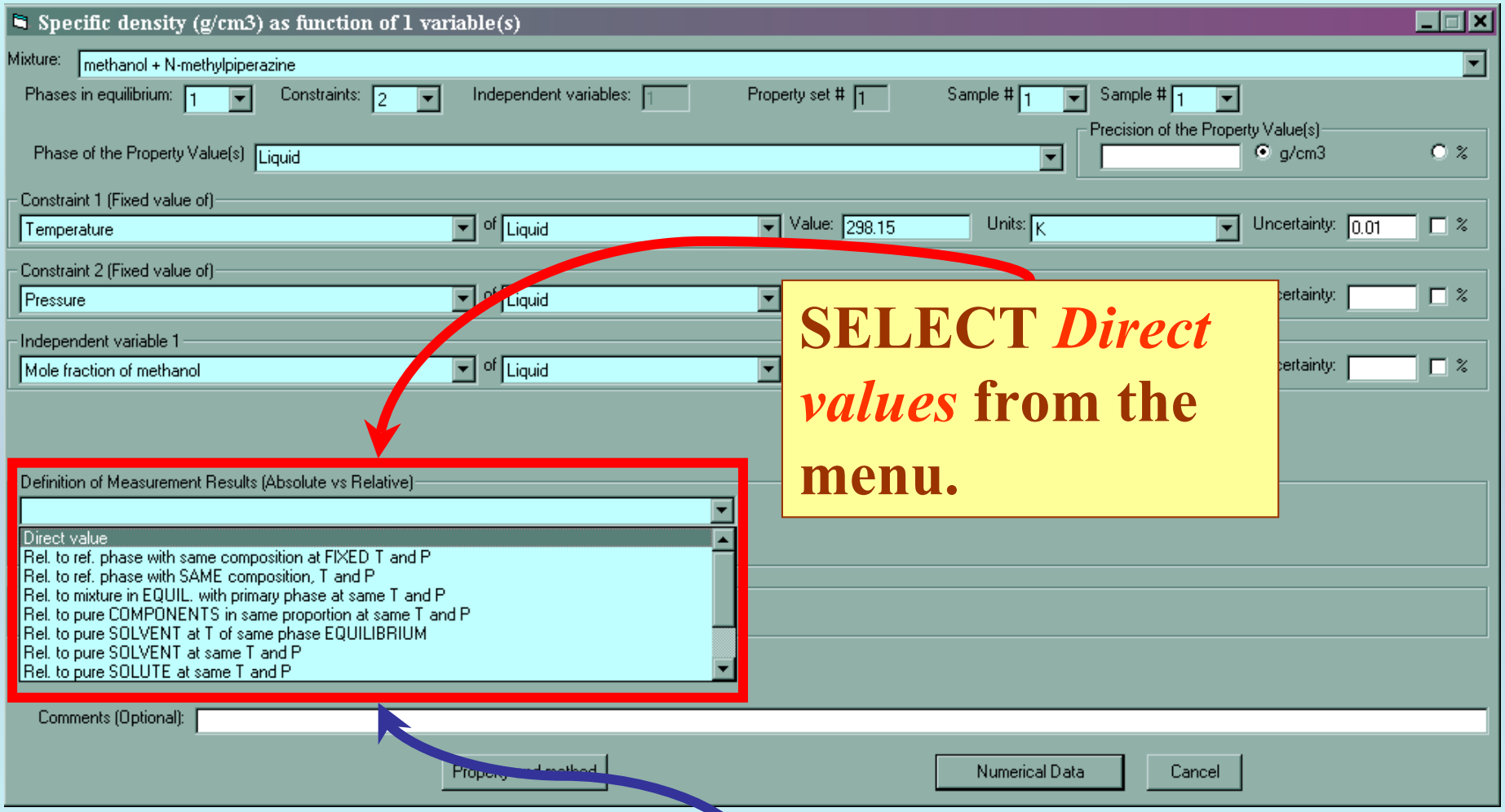


Capture of precisions, if known



NOTE: Only the precision of temperature was provided by the authors in this example.

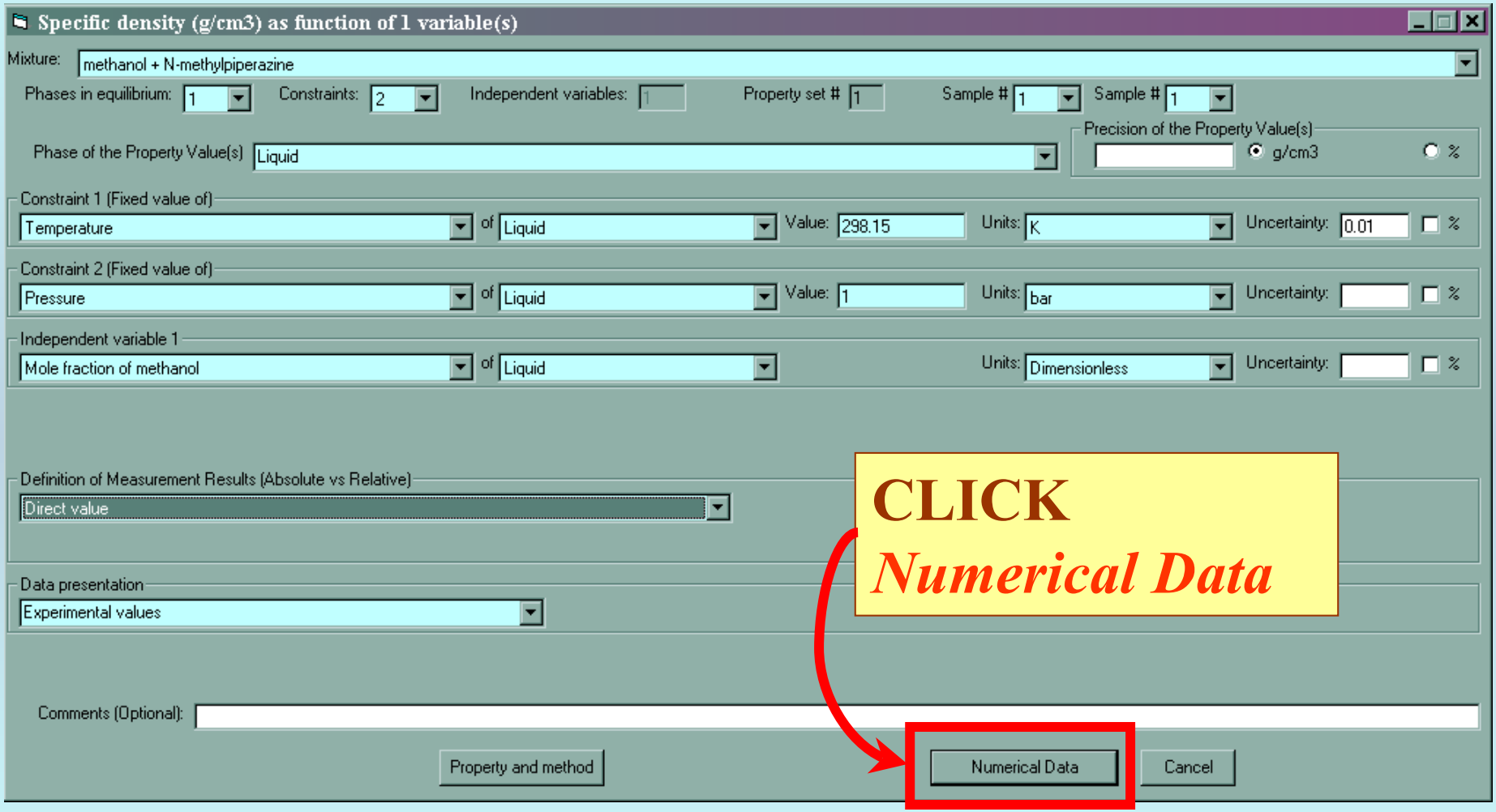
Define results: Absolute vs Relative

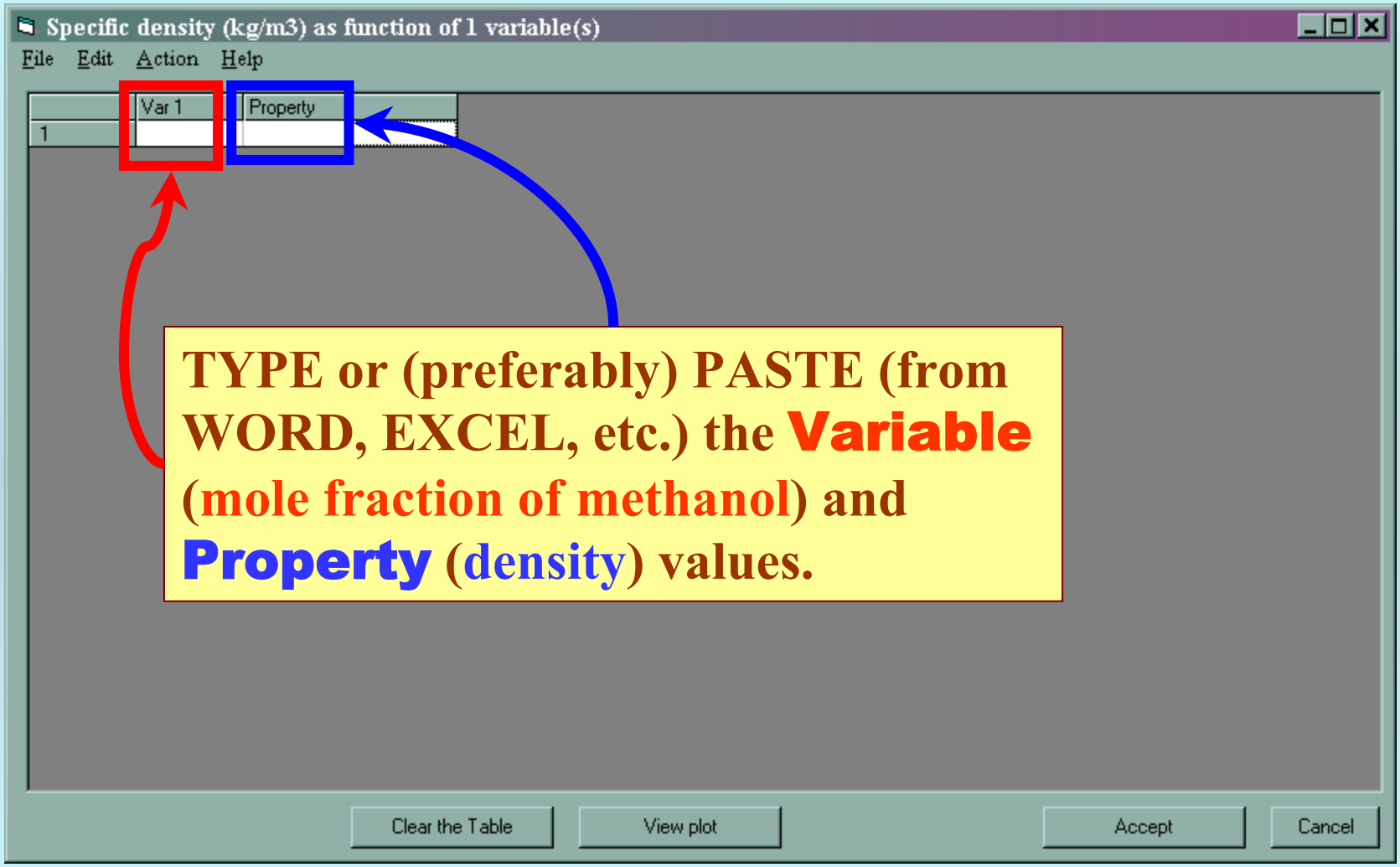


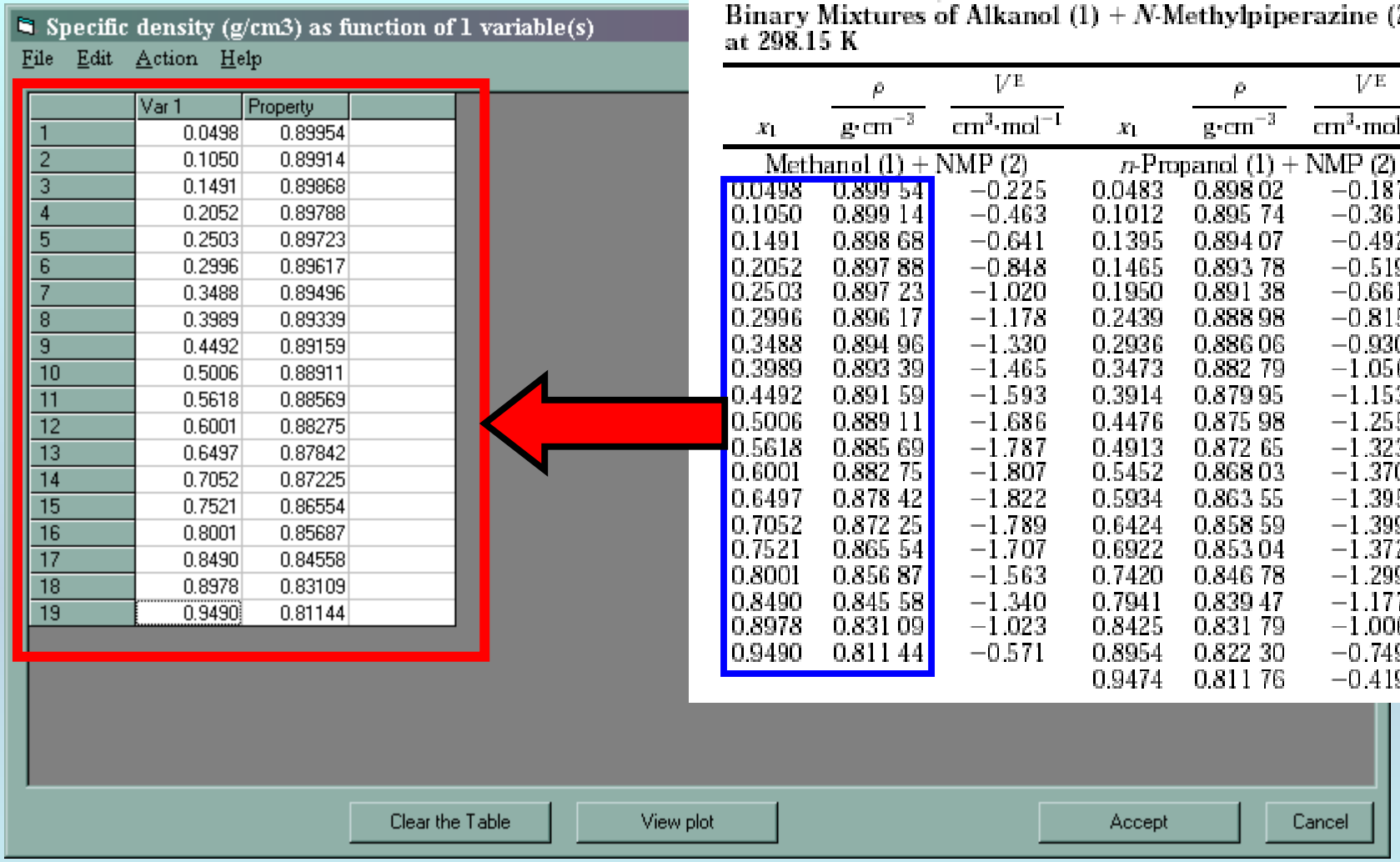
SELECT *Direct values* from the menu.

NOTE: Other options are typically for data reported as relative values (e.g., relative to the density of the pure solovent). These are not common.

Form is complete...




Specific density (kg/m3) as function of 1 variable(s)
File Edit Action Help
Var 1
Property
1
TYPE or (preferably) PASTE (from WORD, EXCEL, etc.) the Variable (mole fraction of methanol) and Property (density) values.
Clear the Table
View plot
Accept
Cancel



	Var 1	Property	
1	0.0498	0.89954	
2	0.1050	0.89914	
3	0.1491	0.89868	
4	0.2052	0.89788	
5	0.2503	0.89723	
6	0.2996	0.89617	
7	0.3488	0.89496	
8	0.3989	0.89339	
9	0.4492	0.89159	
10	0.5006	0.88911	
11	0.5618	0.88569	
12	0.6001	0.88275	
13	0.6497	0.87842	
14	0.7052	0.87225	
15	0.7521	0.86554	
16	0.8001	0.85687	
17	0.8490	0.84558	
18	0.8978	0.83109	
19	0.9490	0.81144	

Table 3. Density ρ and Excess Molar Volume V^E for Binary Mixtures of Alkanol (1) + *N*-Methylpiperazine (2) at 298.15 K

x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}	x_1	ρ / g·cm^{-3}	V^E / cm^3·mol^{-1}
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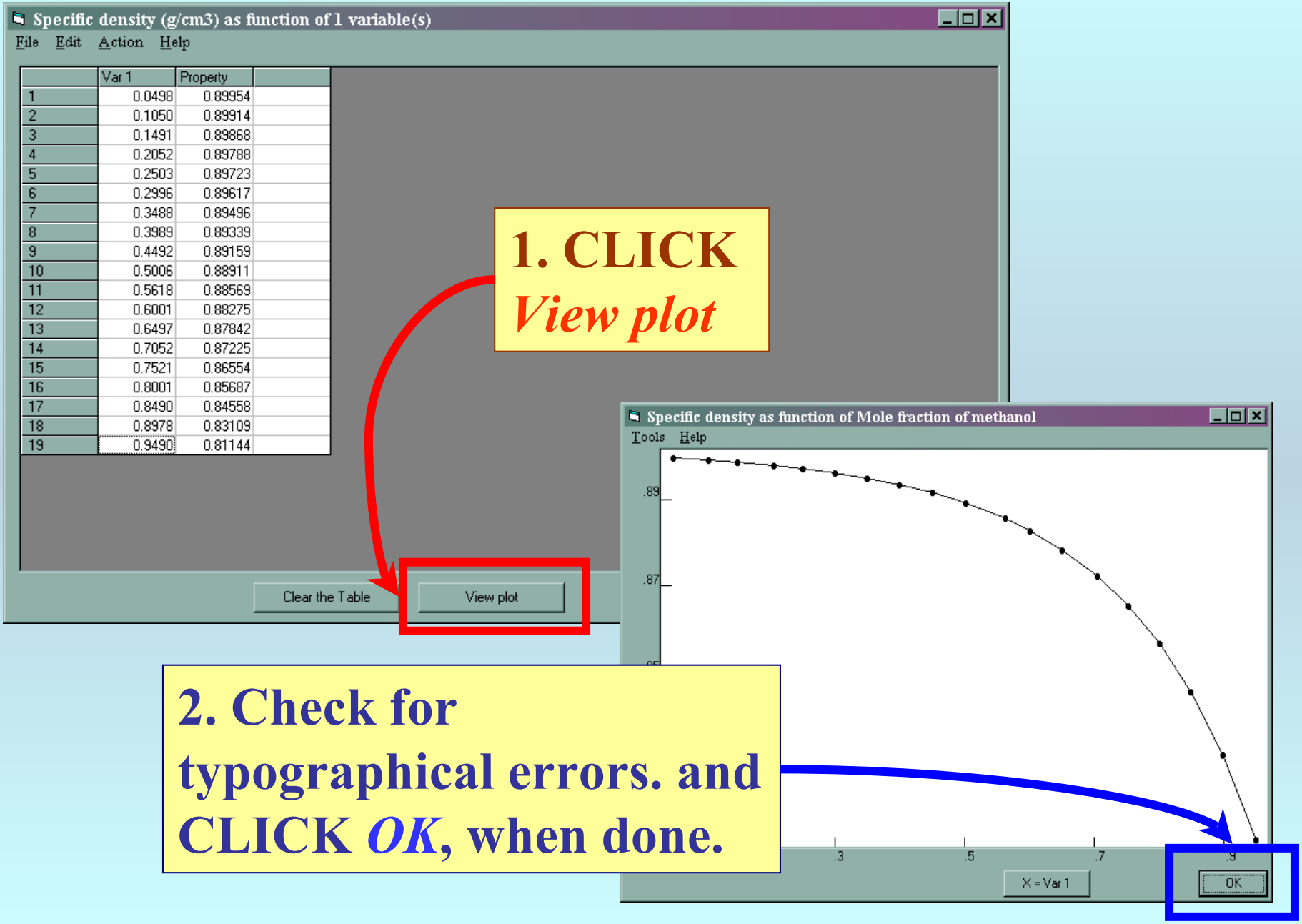
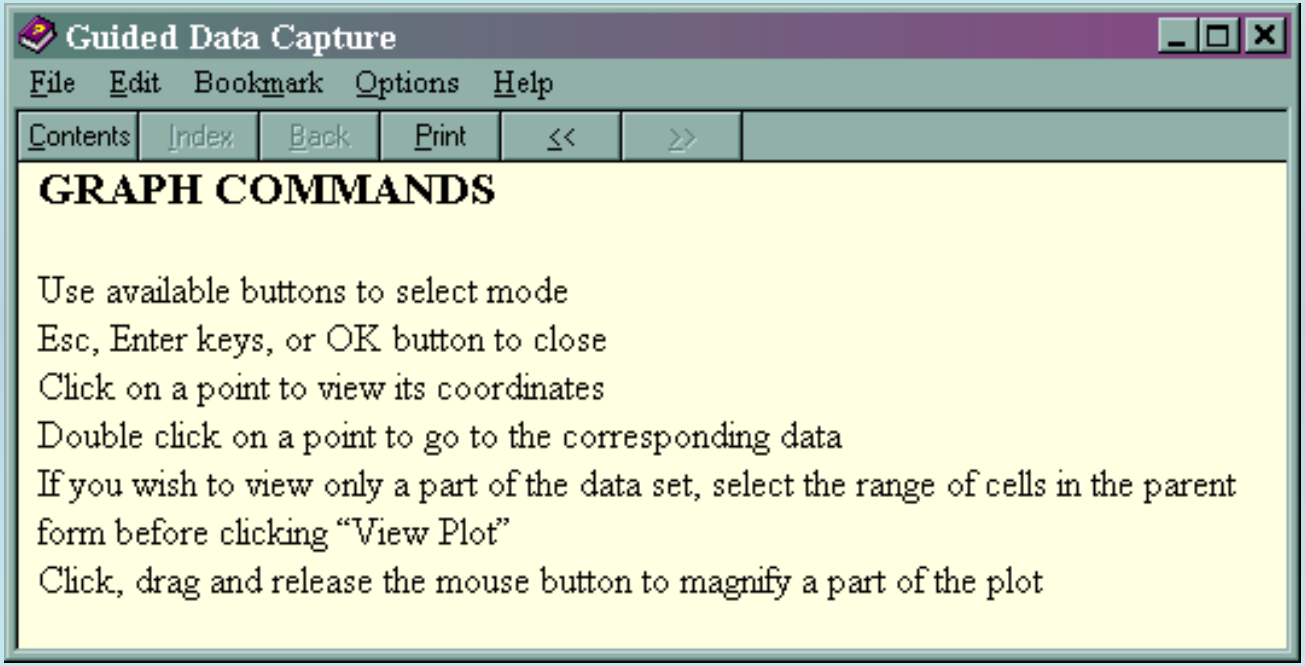
0.9490	0.811 44	−0.571	0.8954	0.822 30	−0.749
			0.9474	0.811 76	−0.419

***Type* or (preferably) *Paste* from WORD, EXCEL, etc.**

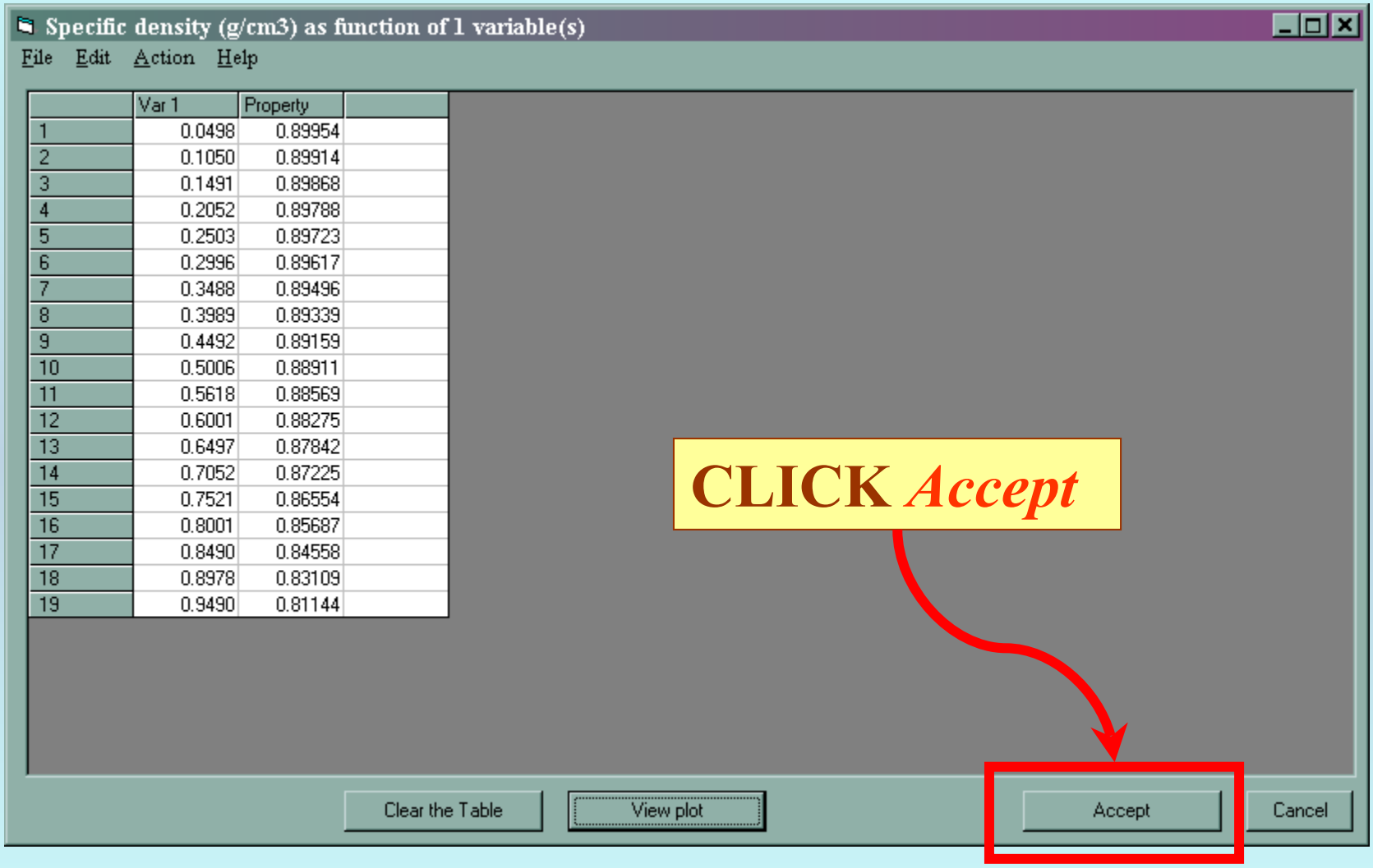
Graphical check for typographical errors

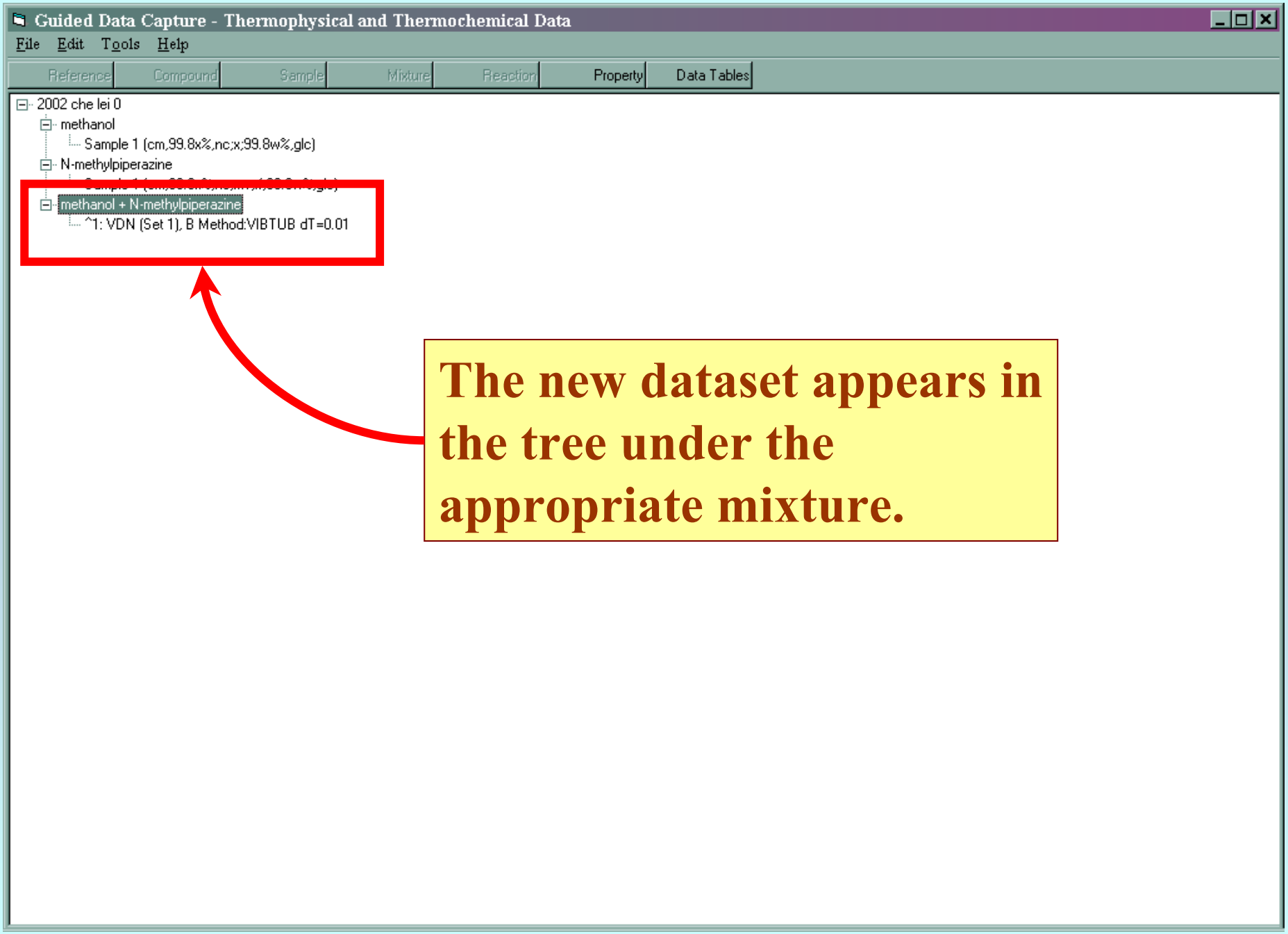


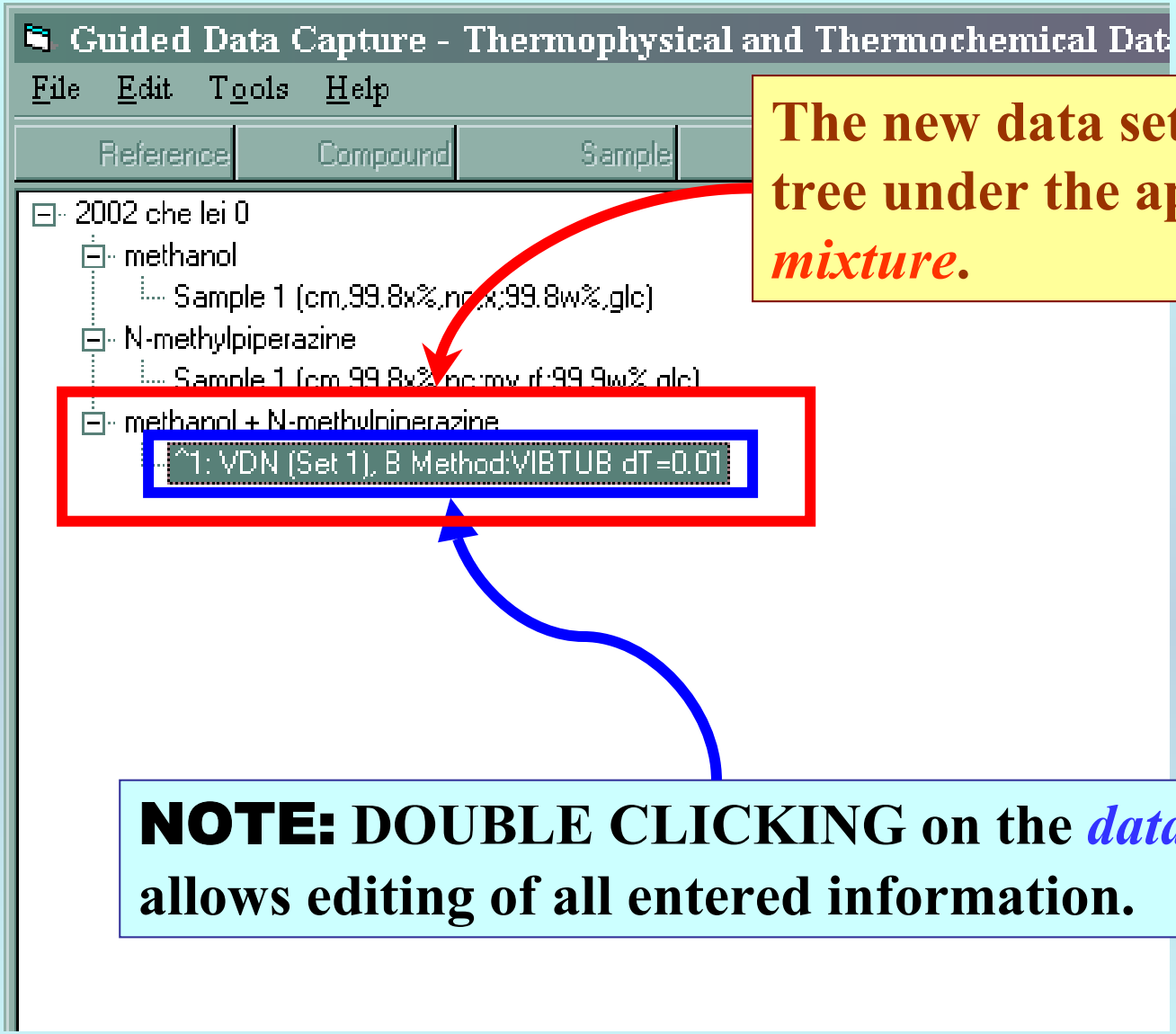
NOTE: The plots have several useful features. See the *HELP* screen on the plot.



Final acceptance




Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property Data Tables
2002 che lei 0
methanol
Sample 1 (cm,99.8x%,nc;x;99.8w%,glc)
N-methylpiperazine
methanol + N-methylpiperazine
^1: VDN (Set 1), B Method:VIBTUB dT=0.01
The new dataset appears in the tree under the appropriate mixture.



The new data set 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.**