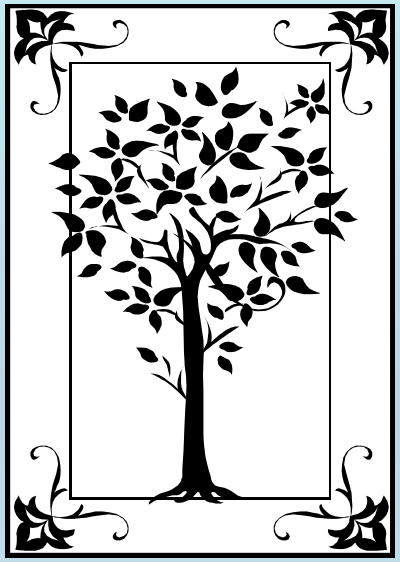
METADATA AND NUMERICAL DATA CAPTURE:
Speed of Sound
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components**
Speed of Sound
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:

312 *J. Chem. Eng. Data* 2001, *46,* 312−316

Temperature Dependence of Densities and Speeds of Sound of Nitromethane + Butanol Isomers in the Range (288.15−308.15) K

Jacobo Troncoso, Clara A. Tovar, Claudio A. Cerdeiriña, Enrique Carballo, and Luís Romaní*

Departamento de Física Aplicada, Universidad de Vigo, Facultad de Ciencias del Campus de Ourense, 32004 Ourense, Spain

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Densities and speeds of sound of the systems nitromethane + 1-butanol, nitromethane + 2-methyl-propan-1-ol, and nitromethane + 2-butanol were measured in the temperature range (288.15−308.15) K. Excess molar volumes are discussed and compared with those of other systems polar fluid + alcohol founded in the literature.

Speeds of Sound for the binary system **2,2,2-trifluoroethanol + quinoline** at p = 101.3 kPa and various temperatures

Table 3. Selected Data of Densities ρ and Speeds of Sound u for the Studied Mixtures

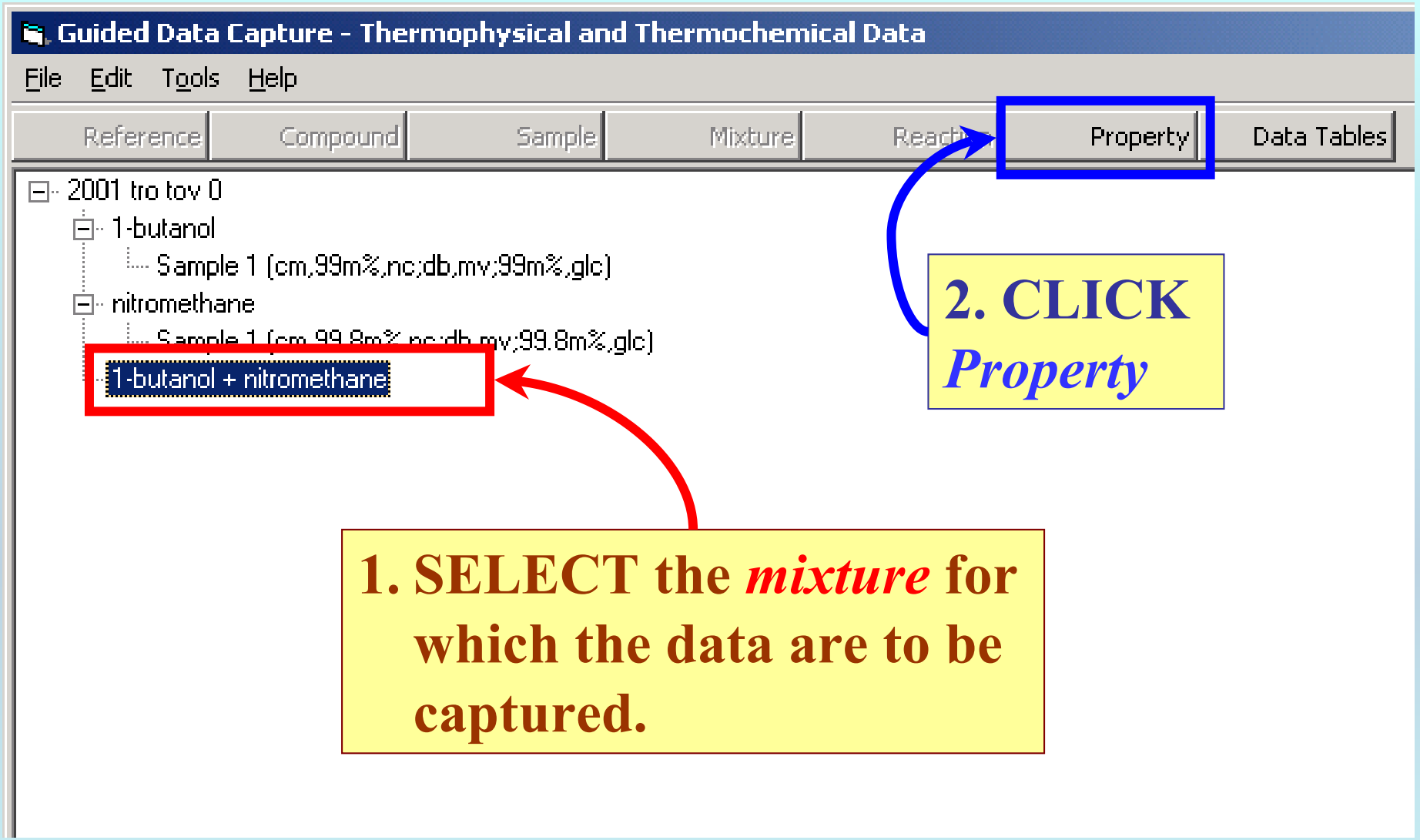
	ρ/g·cm^{-3}					u/m·s^{-1}				
x	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K
				x Nitromethane + (1 − x) 1-Butanol						
0.056 70		0.82000	0.816 09	0.812 08	0.808 05		1255.86	1238.64	1221.53	1205.03
0.103 78		0.82925	0.825 17	0.821 04	0.816 88		1255.12	1238.01	1220.76	1203.96
0.197 35		0.84872	0.844 44	0.840 02	0.835 66		1254.38	1236.86	1218.87	1202.62
0.290 57		0.87012	0.865 62	0.860 99	0.856 34		1253.87	1236.36	1219.03	1201.74
0.346 86		0.88404	0.879 43	0.874 78	0.870 13		1254.30	1237.41	1218.59	1202.14
0.425 91		0.90500	0.900 05	0.895 04	0.890 00		1253.82	1236.96	1219.93	1203.02
0.482 52		0.92115	0.916 01	0.910 81	0.905 62		1254.03	1237.24	1221.17	1204.63
0.524 56		0.93390	0.928 61	0.923 30	0.917 98		1255.68	1238.16	1222.92	1206.35
0.559 49		0.94502	0.939 63	0.934 24	0.928 78		1256.76	1240.56	1224.36	1208.18
0.587 64		0.95421	0.948 73	0.943 20	0.937 71		1257.09	1241.01	1225.21	1209.97
0.689 09		0.98996	0.984 27	0.978 52	0.972 77		1267.10	1251.14	1235.51	1219.22
0.750 78		1.01394	1.008 07	1.002 18	0.996 29		1277.35	1260.39	1244.39	1227.41
0.852 46		1.05815	1.051 89	1.045 59	1.039 26		1300.15	1282.17	1264.12	1246.13
0.946 35		1.10580	1.099 35	1.092 86	1.086 02		1326.53	1307.10	1287.76	1268.97

This data set is considered here.

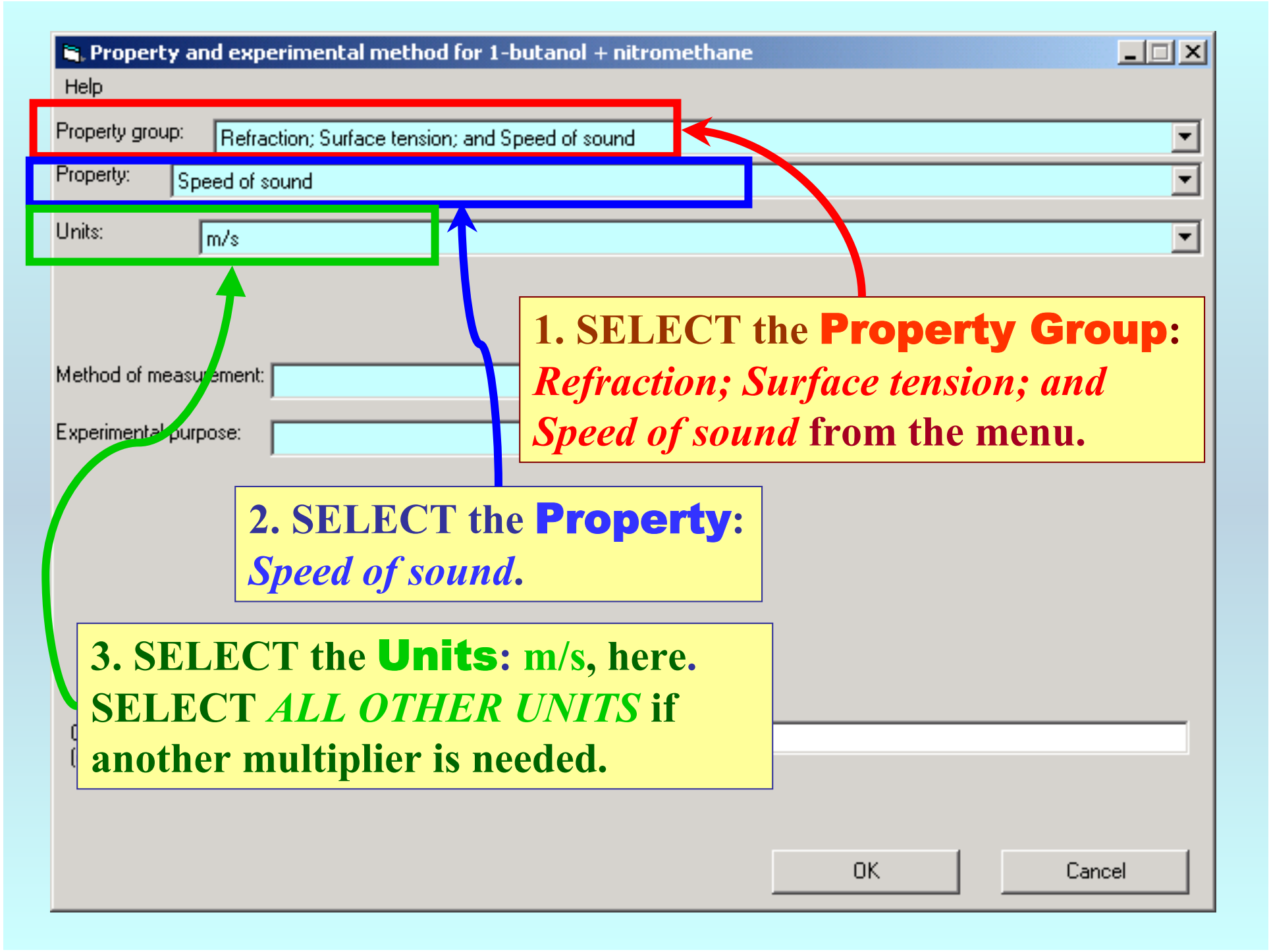
Experimental Method Info:

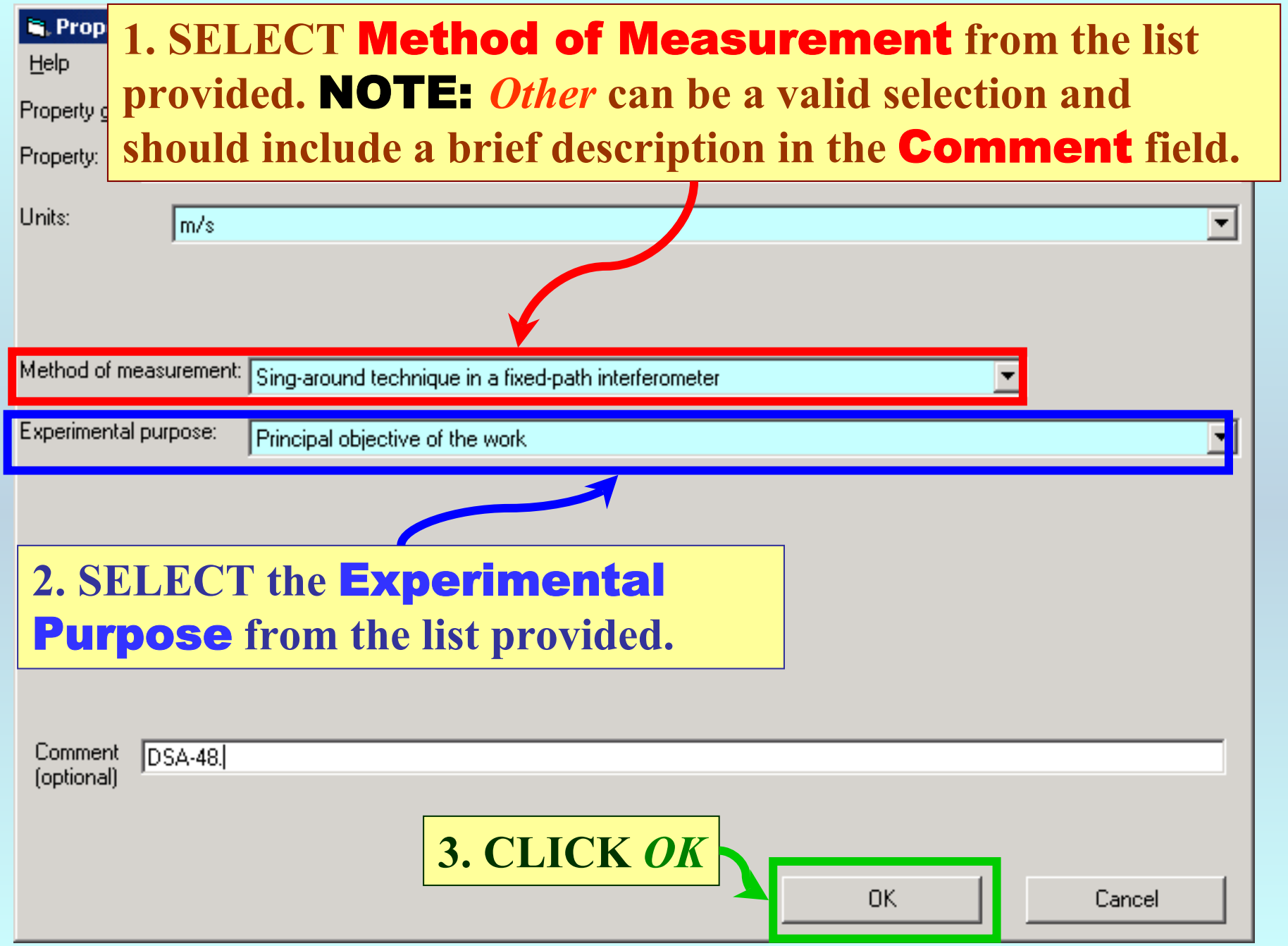
Densities ρ and speeds of sound u of the pure components and of the binary mixtures were measured using a DSA-48 densimeter and sound analyzer. This apparatus, con-

The temperature was controlled through a solid-state thermostat that uses the Peltier effect, and the precision in the temperature was ±0.005 K. The precision is estimated to be about $\pm 2 \times 10^{-5}$ for mole fraction x, $\pm 1 \times 10^{-5}$ g·cm^{-3} for ρ, and ±0.02 m·s^{-1} for u.

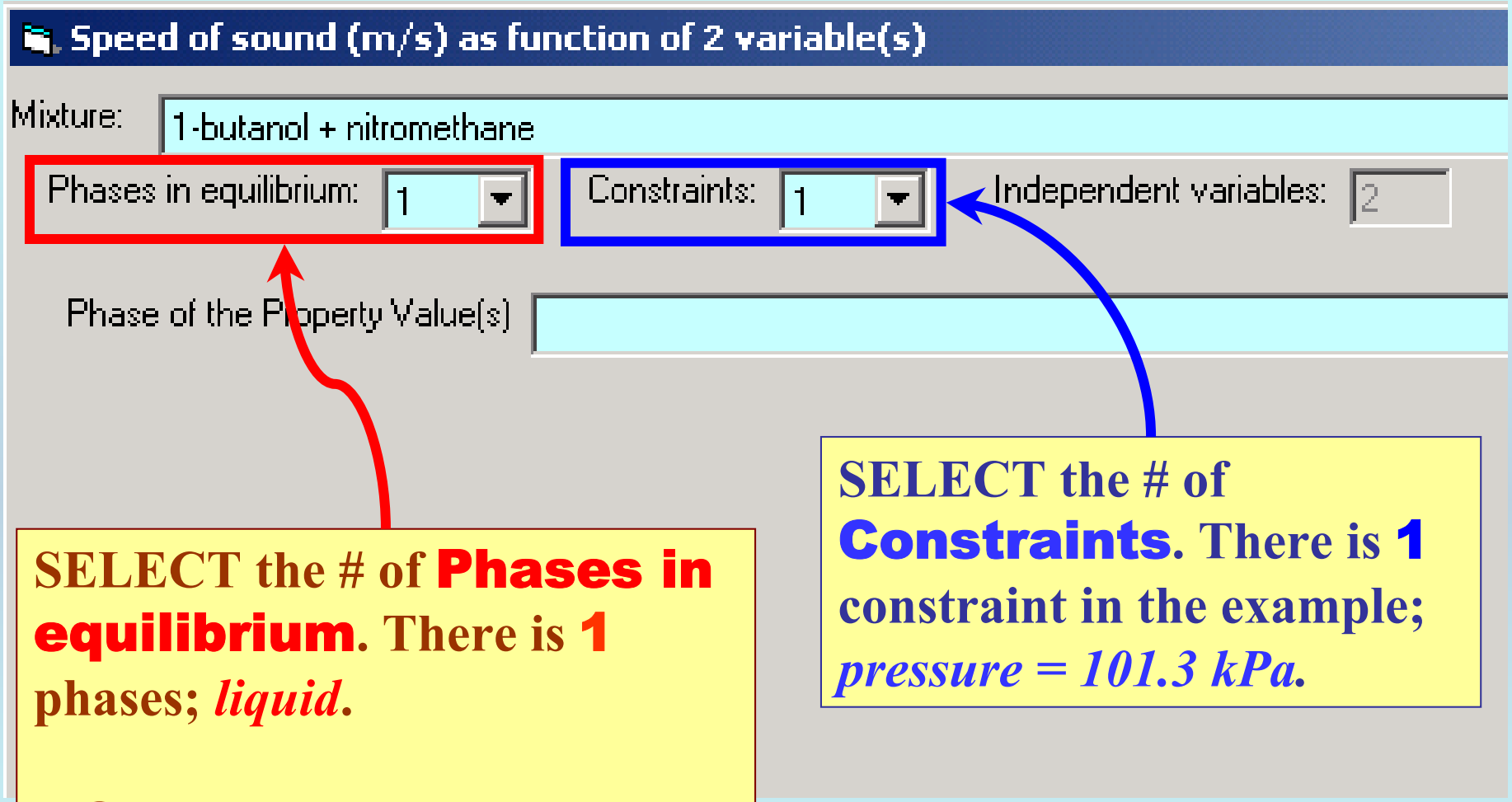


NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for 1-butanol + nitromethane
Help
Property group:
Refraction; Surface tension; and Speed of sound
Property:
Speed of sound
Units:
m/s
Method of measurement:
Experimental purpose:
1. SELECT the Property Group: Refraction; Surface tension; and Speed of sound from the menu.
2. SELECT the Property: Speed of sound.
3. SELECT the Units: m/s, here. SELECT ALL OTHER UNITS if another multiplier is needed.
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.
Help
Property:
Units:
m/s
Method of measurement:
Sing-around technique in a fixed-path interferometer
Experimental purpose:
Principal objective of the work
2. SELECT the Experimental Purpose from the list provided.
Comment (optional)
DSA-48
3. CLICK OK
OK
Cancel

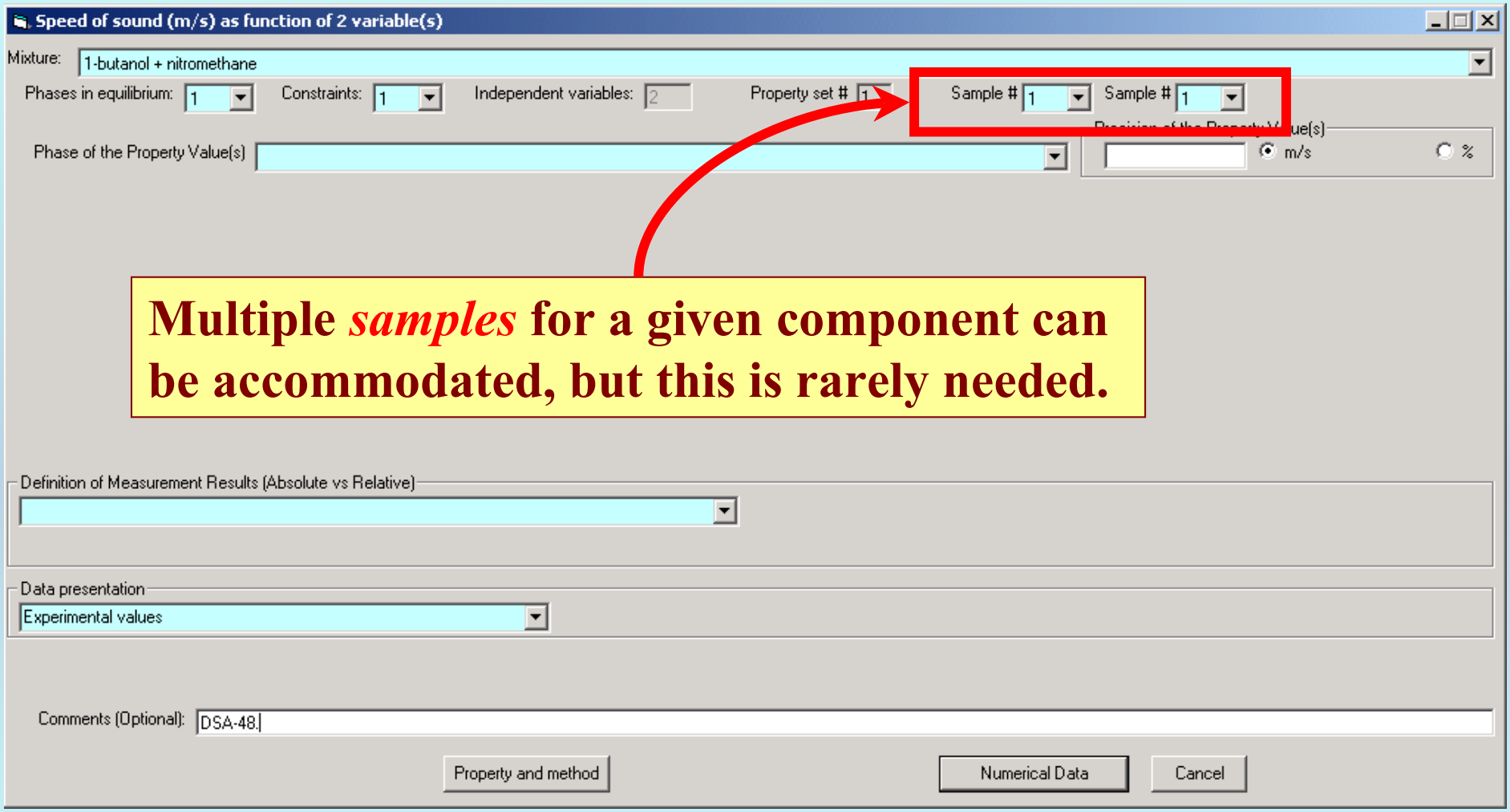
SELECTION of # of Phases in Equilibrium and # of Constraints

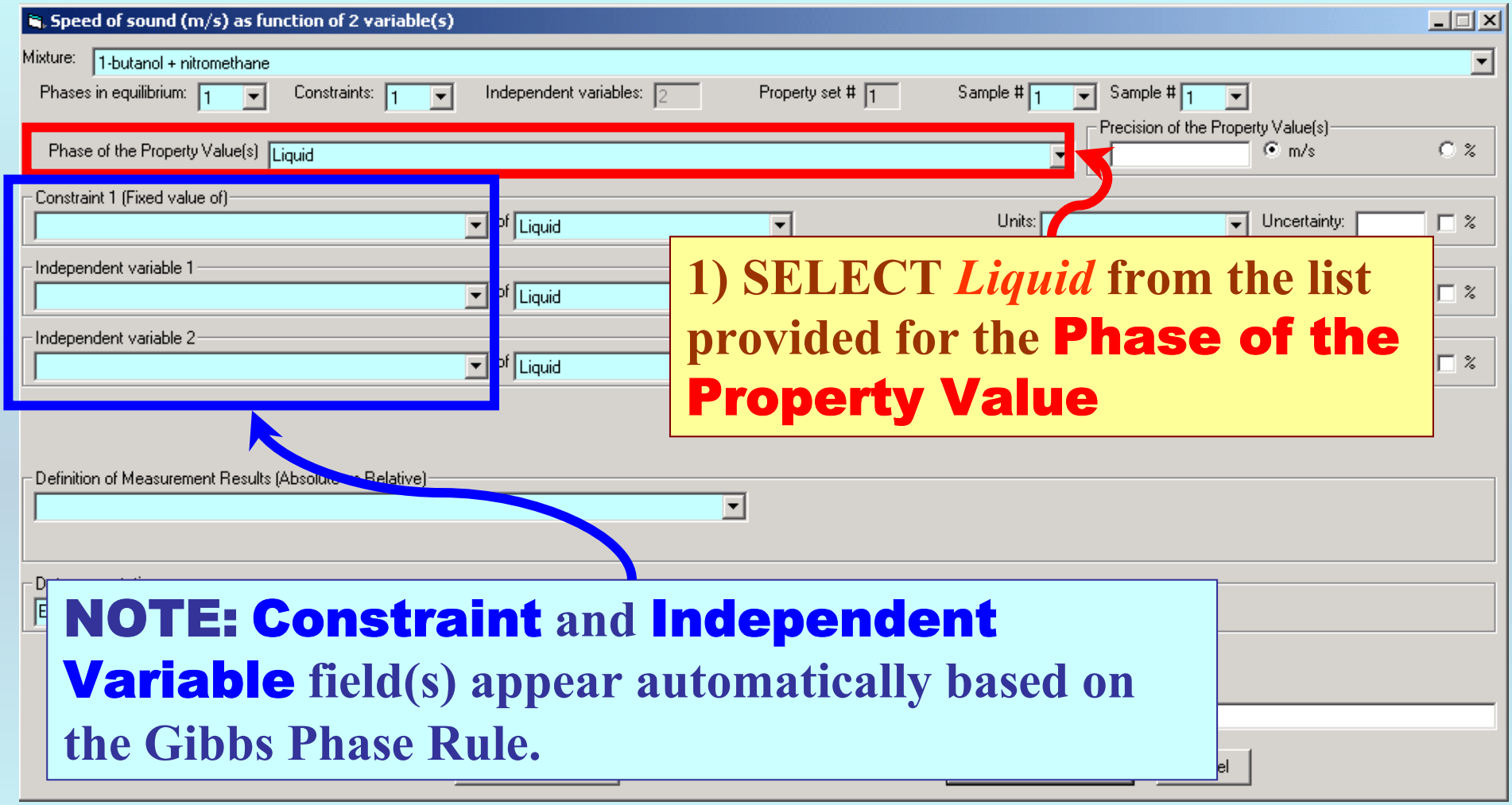


SELECT the # of **Phases in equilibrium**. There is **1** phases; *liquid*.

NOTE: *For "saturation conditions, this value would be 2; liquid & gas)*

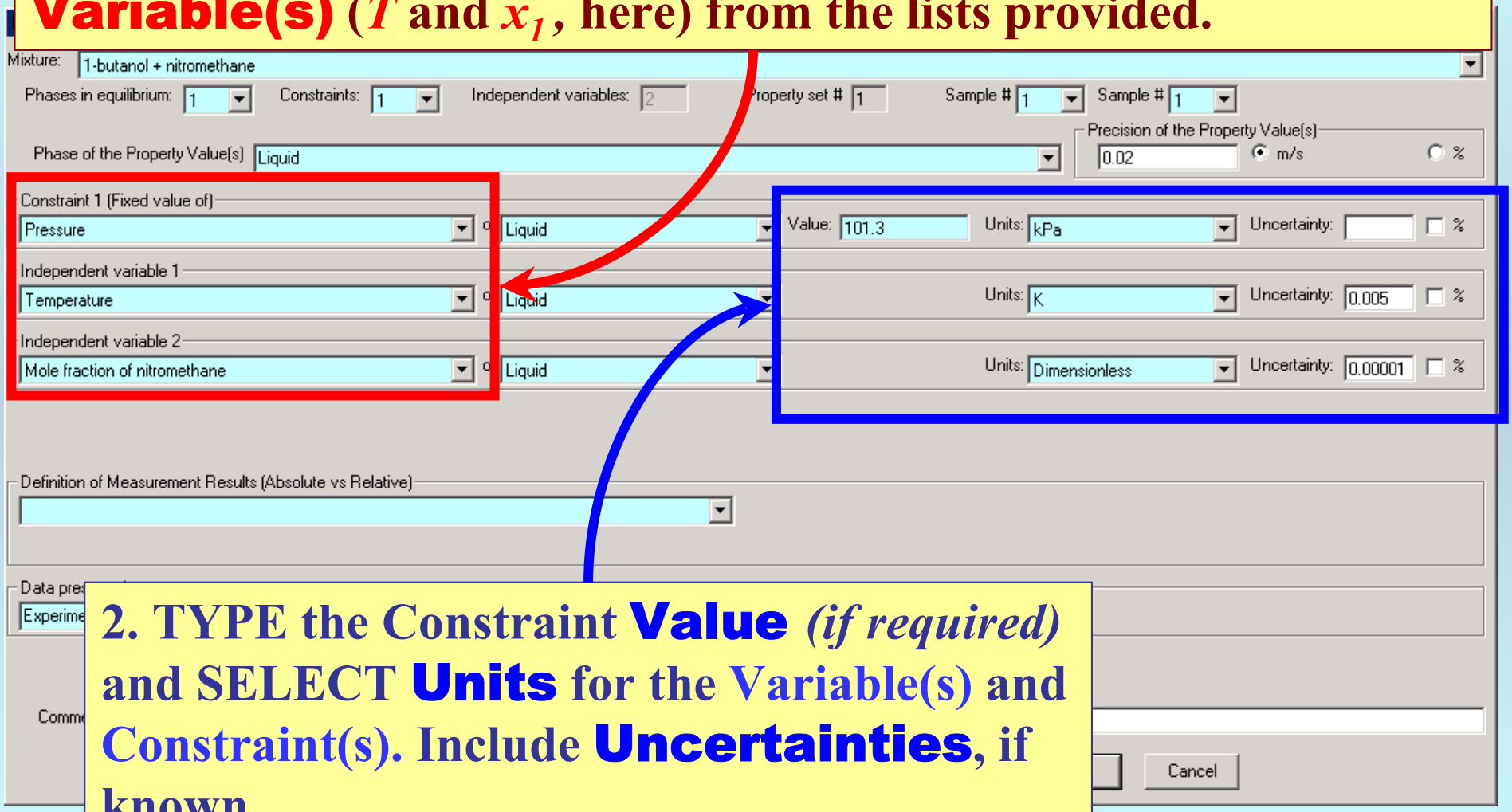
SELECT the # of **Constraints**. There is **1** constraint in the example; *pressure = 101.3 kPa*.


Speed of sound (m/s) as function of 2 variable(s)
Mixture:
1-butanol + nitromethane
Phases in equilibrium:
1
Constraints:
1
Independent variables:
2
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
m/s
%
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):
DSA-48
Property and method
Numerical Data
Cancel


Speed of sound (m/s) as function of 2 variable(s)
Mixture:
1-butanol + nitromethane
Phases in equilibrium:
Constraints:
Independent variables:
Property set #
Sample #
Sample #
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
m/s
%
Constraint 1 (Fixed value of)
Liquid
Units:
Uncertainty:
Independent variable 1
Liquid
Independent variable 2
Liquid
Definition of Measurement Results (Absolute - Relative)
1) SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

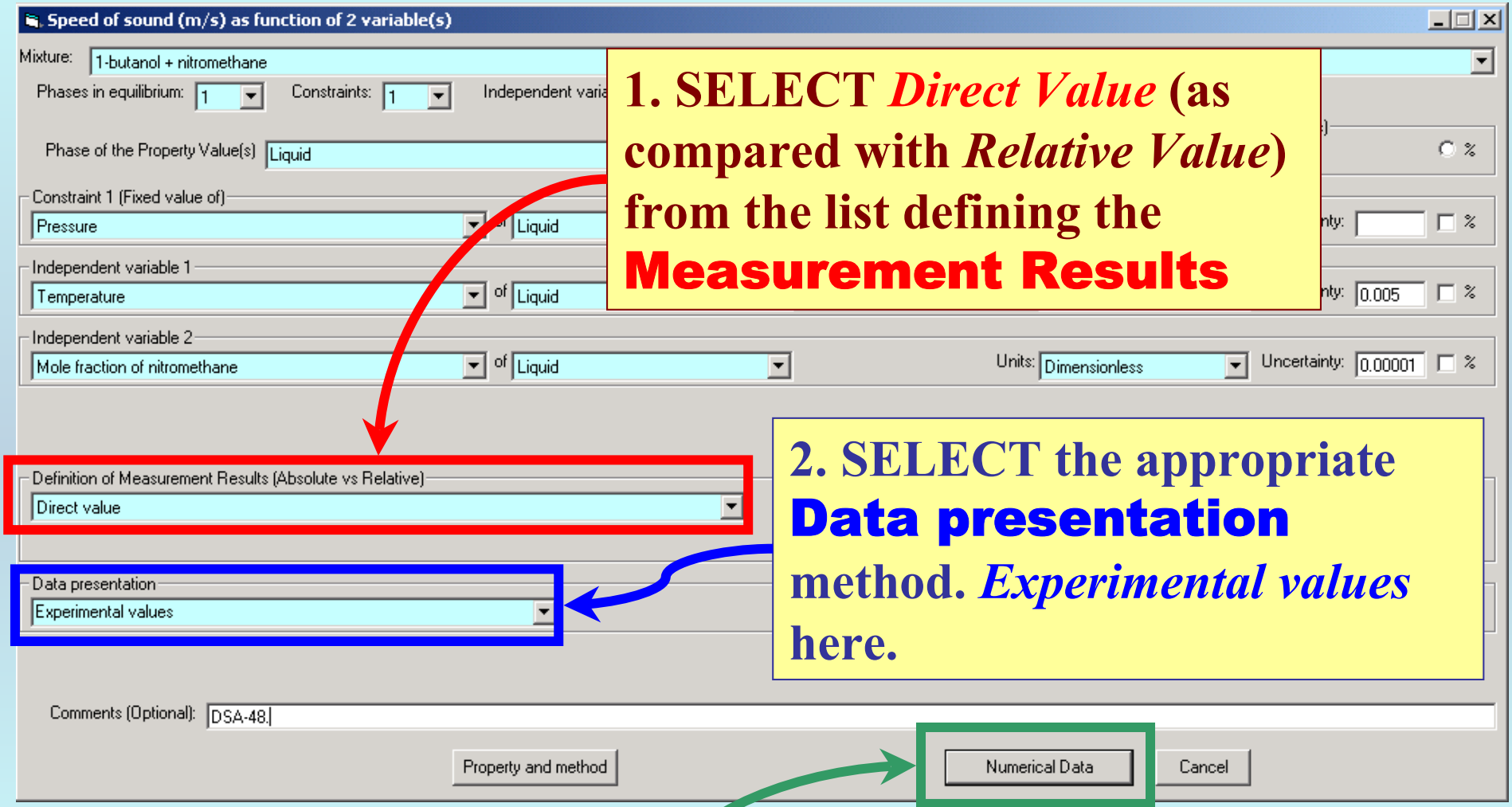
Specification of constraints, constraint values, and constraint units

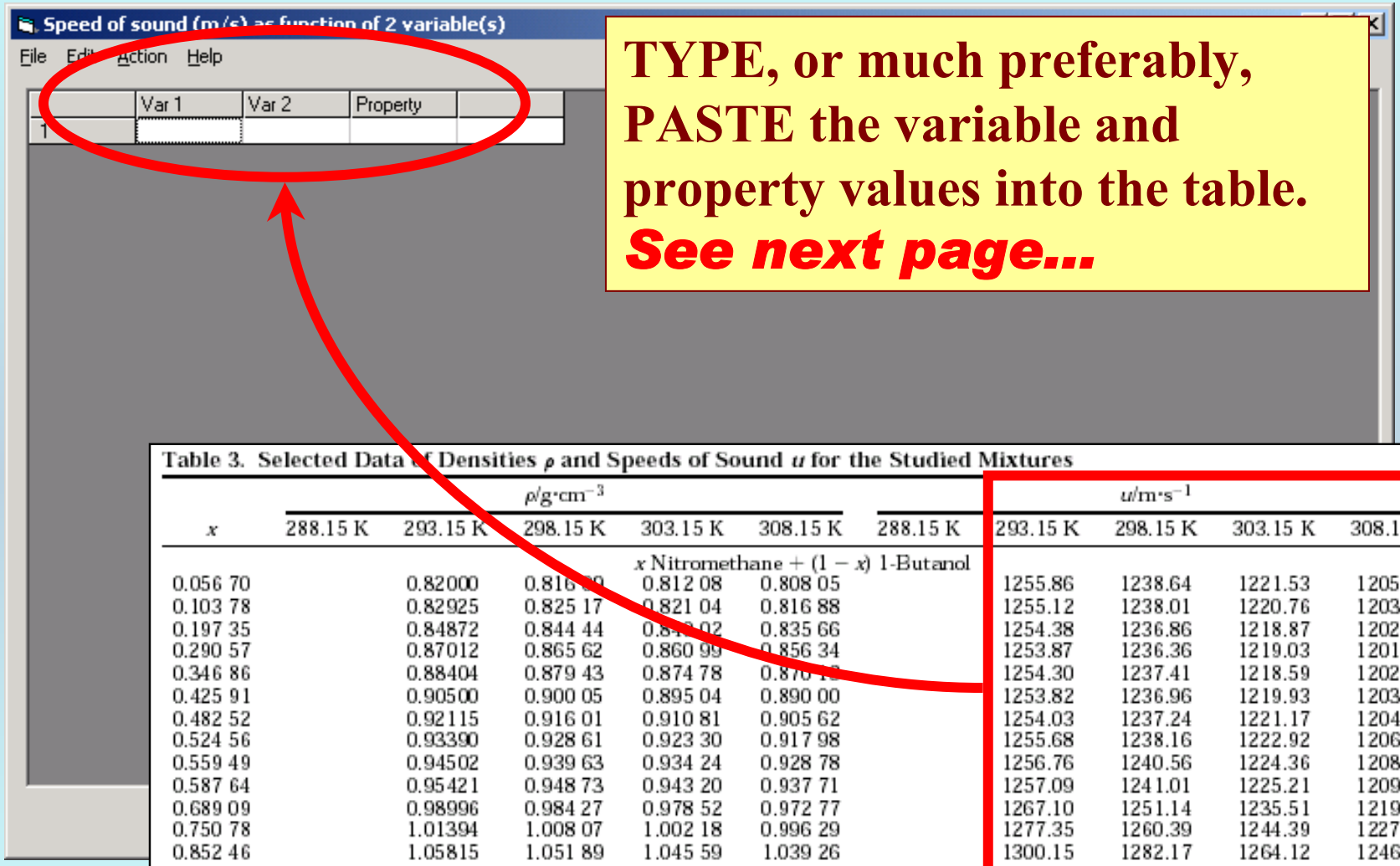
1. SELECT the Constraint(s) (*p* here) and the Independent Variable(s) (*T* and x_1, here) from the lists provided.



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

Measurement definition and Data presentation





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

See next page...

Table 3. Selected Data of Densities ρ and Speeds of Sound u for the Studied Mixtures

	ρ/g·cm^{-3}					u/m·s^{-1}				
x	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K
				x Nitromethane + (1 − x) 1-Butanol						
0.056 70		0.82000	0.816 [illegible]	0.812 08	0.808 05		1255.86	1238.64	1221.53	1205.03
0.103 78		0.82925	0.825 17	0.821 04	0.816 88		1255.12	1238.01	1220.76	1203.96
0.197 35		0.84872	0.844 44	0.84[illegible]02	0.835 66		1254.38	1236.86	1218.87	1202.62
0.290 57		0.87012	0.865 62	0.860 99	0.856 34		1253.87	1236.36	1219.03	1201.74
0.346 86		0.88404	0.879 43	0.874 78	0.870 [illegible]		1254.30	1237.41	1218.59	1202.14
0.425 91		0.90500	0.900 05	0.895 04	0.890 00		1253.82	1236.96	1219.93	1203.02
0.482 52		0.92115	0.916 01	0.910 81	0.905 62		1254.03	1237.24	1221.17	1204.63
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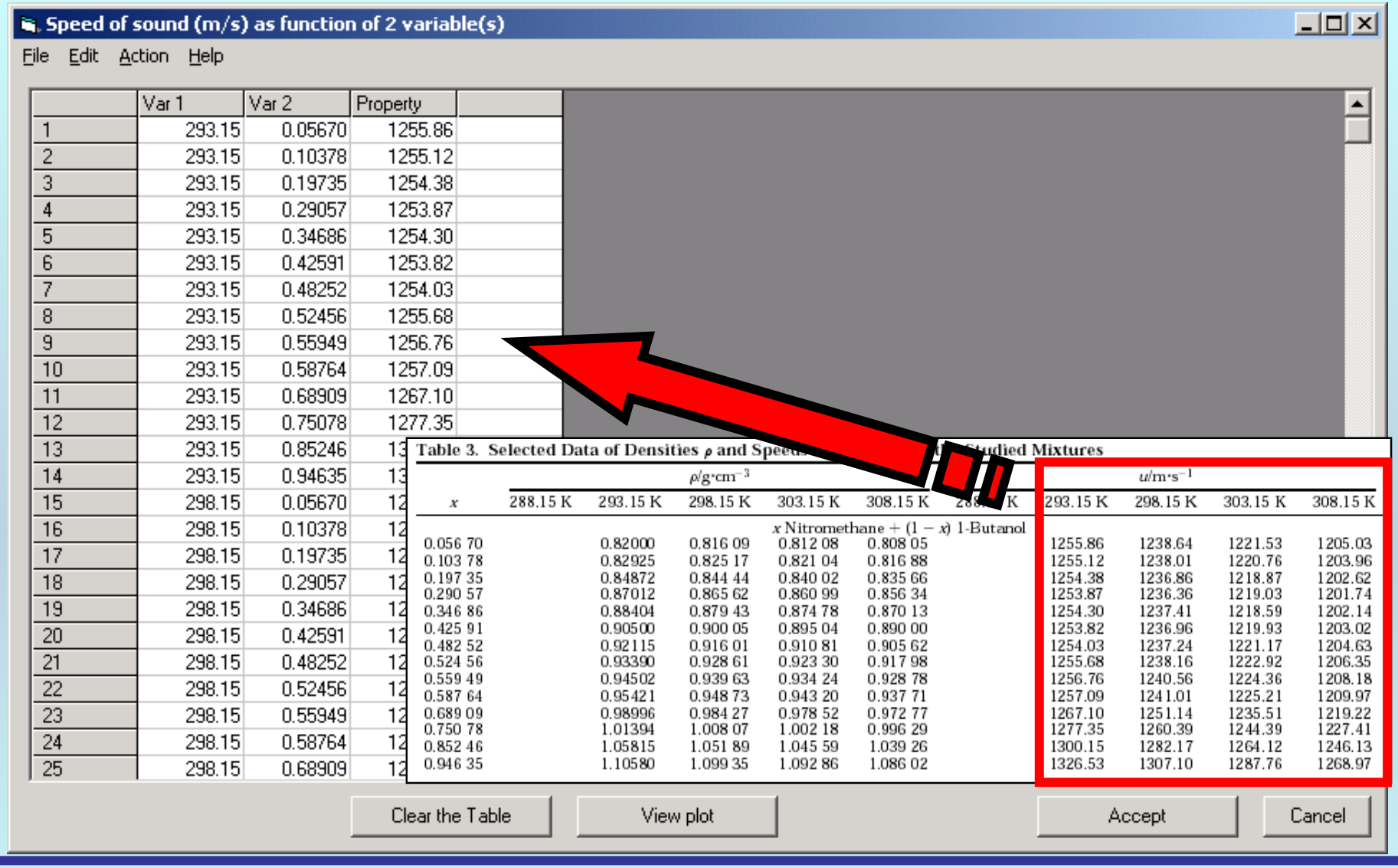
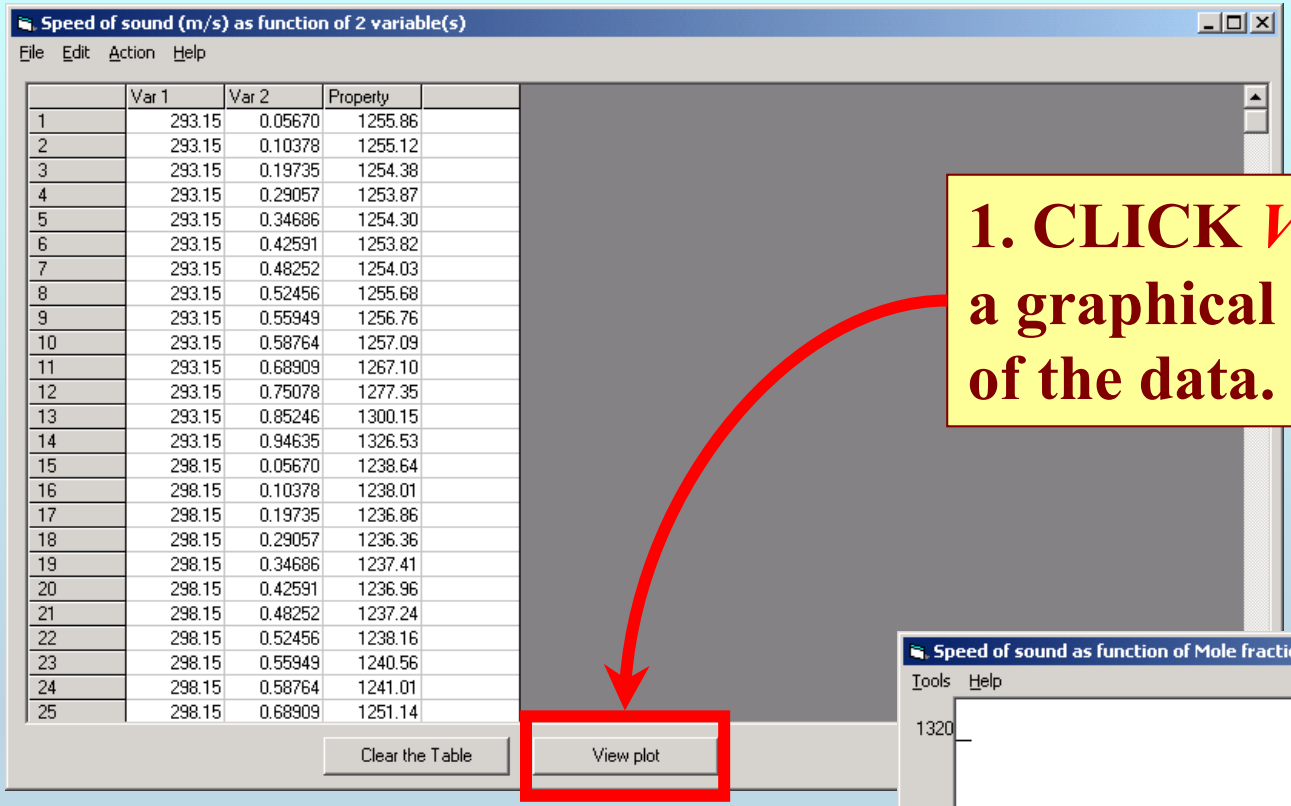
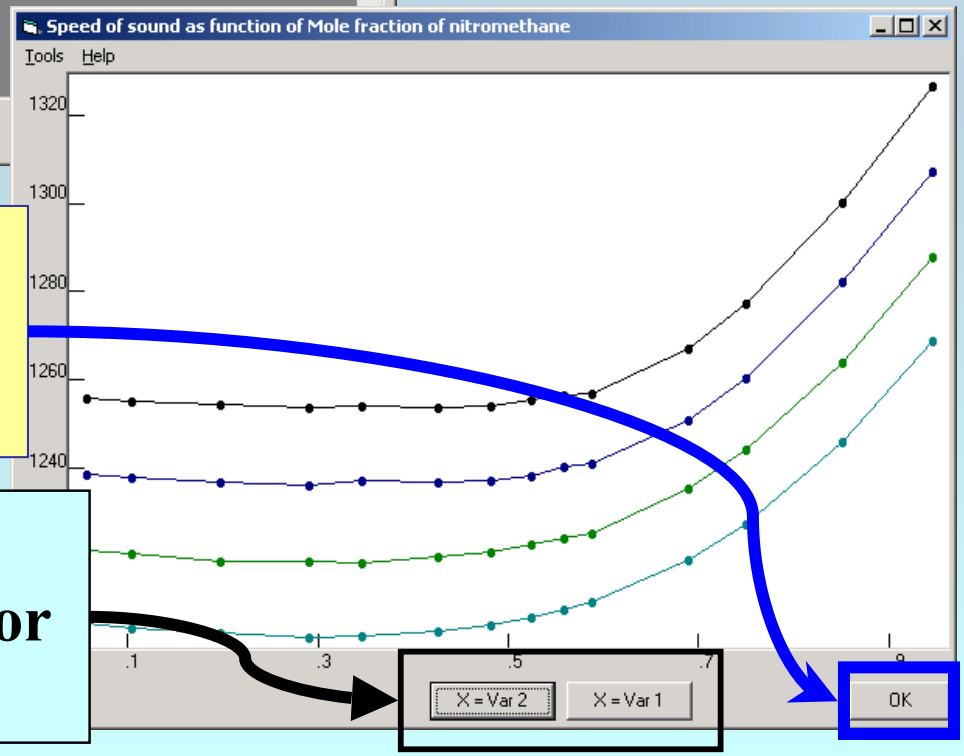
0.689 09		0.98996	0.984 27	0.978 52	0.972 77		1267.10	1251.14	1235.51	1219.22
0.750 78		1.01394	1.008 07	1.002 18	0.996 29		1277.35	1260.39	1244.39	1227.41
0.852 46		1.05815	1.051 89	1.045 59	1.039 26		1300.15	1282.17	1264.12	1246.13
0.946 35		1.10580	1.099 35	1.092 86	1.086 02		1326.53	1307.10	1287.76	1268.97



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.)

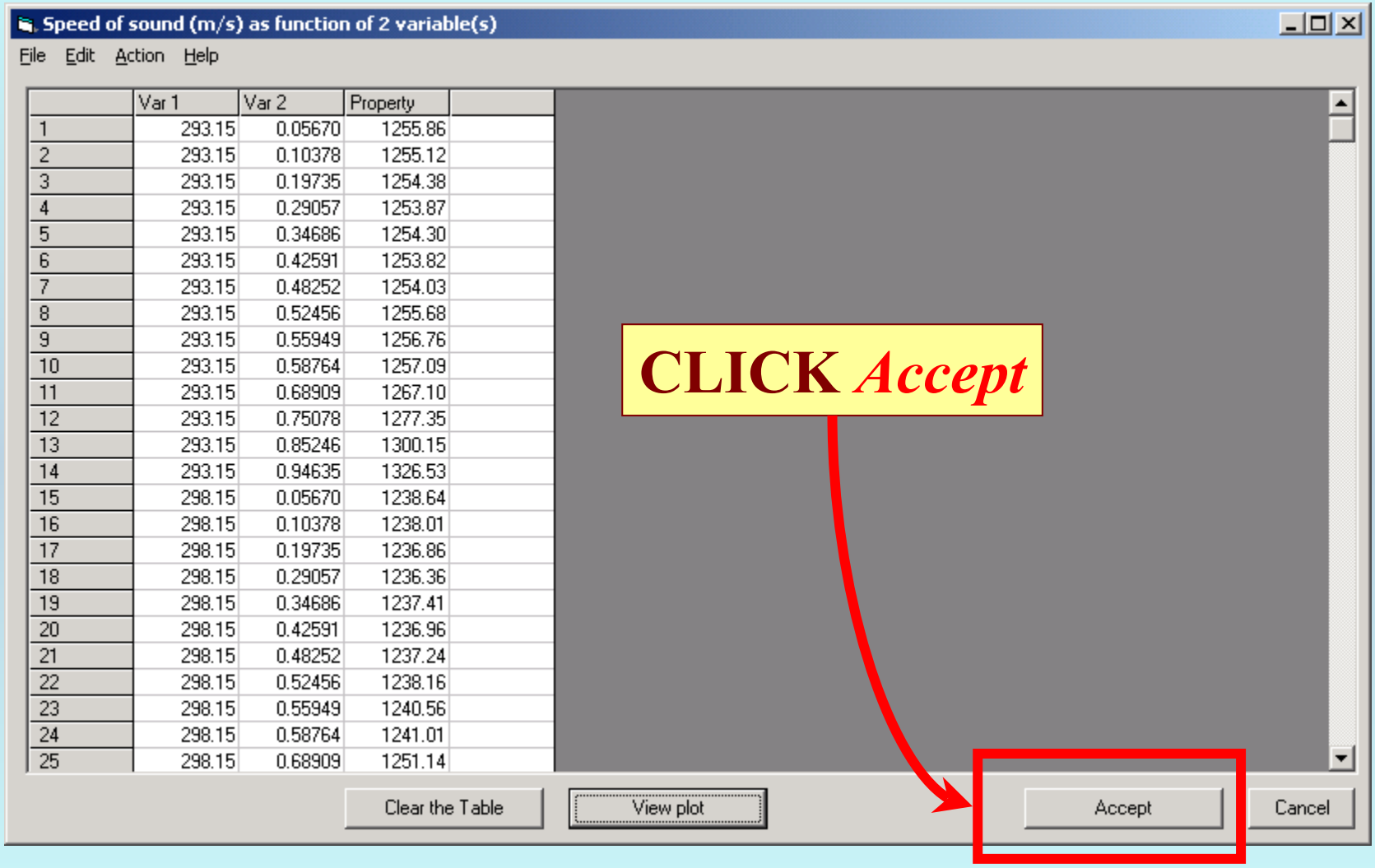


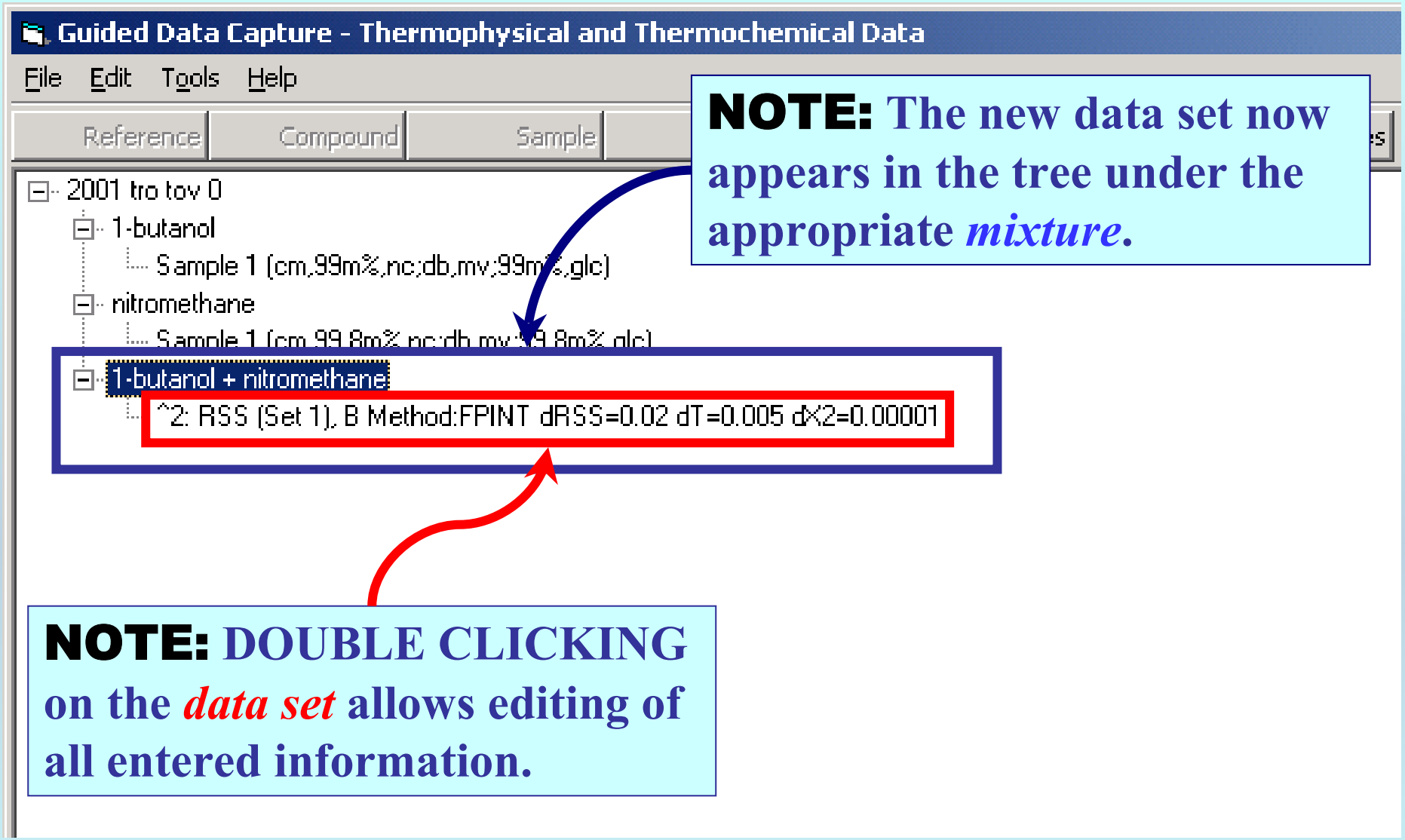
1. CLICK *View plot* to see a graphical representation of the data.



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

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


Speed of sound (m/s) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 293.15 0.05670 1255.86
2 293.15 0.10378 1255.12
3 293.15 0.19735 1254.38
4 293.15 0.29057 1253.87
5 293.15 0.34686 1254.30
6 293.15 0.42591 1253.82
7 293.15 0.48252 1254.03
8 293.15 0.52456 1255.68
9 293.15 0.55949 1256.76
10 293.15 0.58764 1257.09
11 293.15 0.68909 1267.10
12 293.15 0.75078 1277.35
13 293.15 0.85246 1300.15
14 293.15 0.94635 1326.53
15 298.15 0.05670 1238.64
16 298.15 0.10378 1238.01
17 298.15 0.19735 1236.86
18 298.15 0.29057 1236.36
19 298.15 0.34686 1237.41
20 298.15 0.42591 1236.96
21 298.15 0.48252 1237.24
22 298.15 0.52456 1238.16
23 298.15 0.55949 1240.56
24 298.15 0.58764 1241.01
25 298.15 0.68909 1251.14
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample
2001 tro tov 0
1-butanol
Sample 1 (cm,99m%,nc;db,mv;99m%,glc)
nitromethane
1-butanol + nitromethane
^2: RSS (Set 1), B Method:FPINT dRSS=0.02 dT=0.005 dX2=0.00001
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.**