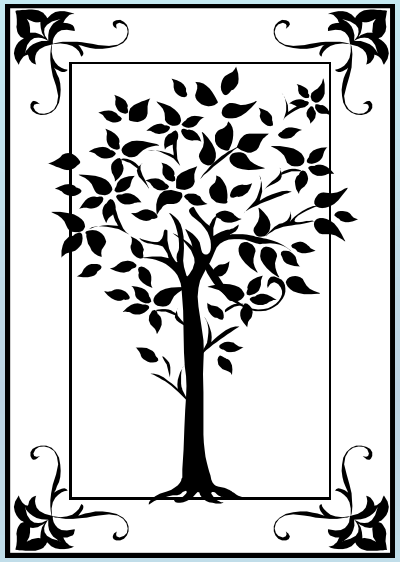
METADATA AND NUMERICAL DATA CAPTURE:
DENSITY = f(*T*,*p*,*x*)
2 – Components and 1 Phase

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-components and 1 phase**
DENSITY (kg/m^3)
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*, 233−238

High-Pressure Volumetric Behavior of *x* 1,1,1,2-Tetrafluoroethane + (1 − *x*) 2,5,8,11,14-Pentaoxapentadecane (TEGDME) Mixtures

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This paper reports 1017 new *pVT* measurements of the *x* 1,1,1,2-tetrafluoroethane (HFC-134a) + (1 − *x*) 2,5,8,11,14-pentaoxapentadecane (TEGDME) system for *x* = 0.0, 0.1114, 0.2896, 0.3648, 0.5702, 0.6931, 0.7288, 0.8727, 0.9290, and 1 between 10 and 60 MPa in the temperature range 293.15 K to 373.15 K at 5 MPa and 10 K intervals, respectively. In almost all the measurement range, the density of the pure compressed refrigerant is greater than that of the pure polyether. For temperatures higher than 343.15 K, the isocomposition curves for the mixtures show an intersection point. Similar behavior has been previously found for HFC-134a + triethylene glycol dimethyl ether, carbon dioxide + alkane or toluene systems, and mixtures of R-410A with polyolester lubricants. The excess molar volume is negative over the whole composition range at all temperatures and pressures.

DENSITY = f(*T*, *p*, *x*)

(2 ñ Components)

1,1,1,2-Tetrafluoroethane (HFC 134a) + 2,5,8,11,14-Pentaoxapentadecane (TEGDME)

Table 1. Experimental Values of Densities, ρ, for x HFC-134a + $(1 - x)$ TEGDME at Different Temperatures, T, and Pressures, p

		ρ/(g·cm^{-3}) at the following values of T/K								
x	p/MPa	293.15	303.15	313.15	323.15	333.15	343.15	353.15	363.15	373.15
0	0.1	1.0112	1.0018	0.9925	0.9833	0.9740	0.9648	0.9556	0.9469	0.9375
	5	1.0142	1.0050	0.9959	0.9868	0.9778	0.9687	0.9598	0.9513	0.9423
	10	1.0172	1.0082	0.9992	0.9903	0.9814	0.9726	0.9639	0.9557	0.9468
	15	1.0201	1.0113	1.0025	0.9937	0.9850	0.9764	0.9679	0.9598	0.9511
	20	1.0229	1.0143	1.0055	0.9970	0.9883	0.9800	0.9716	0.9639	0.9552
	25	1.0257	1.0172	1.0086	1.0001	0.9917	0.9835	0.9752	0.9675	0.9593
	30	1.0284	1.0200	1.0116	1.0032	0.9950	0.9869	0.9788	0.9712	0.9631
	35	1.0310	1.0227	1.0144	1.0063	0.9982	0.9901	0.9821	0.9748	0.9669
	40	1.0336	1.0254	1.0172	1.0091	1.0012	0.9932	0.9855	0.9783	0.9704
	45	1.0361	1.0281	1.0201	1.0121	1.0042	0.9963	0.9886	0.9815	0.9739
	50	1.0385	1.0306	1.0226	1.0147	1.0070	0.9993	0.9917	0.9846	0.9771
	55	1.0410	1.0332	1.0252	1.0175	1.0098	1.0023	0.9947	0.9880	0.9805
	60	1.0434	1.0355	1.0278	1.0202	1.0126	1.0050	0.9976	0.9910	0.9838
0.1114	10	1.0315	1.0220	1.0124	1.0031	0.9936	0.9844	0.9752	0.9659	0.9564
	15	1.0345	1.0254	1.0159	1.0067	0.9975	0.9887	0.9794	0.9704	0.9611
	20	1.0375	1.0285	1.0192	1.0103	1.0011	0.9925	0.9834	0.9746	0.9657
	25	1.0405	1.0316	1.0223	1.0136	1.0047	0.9962	0.9872	0.9787	0.9699
	30	1.0433	1.0346	1.0255	1.0169	1.0081	0.9998	0.9911	0.9828	0.9742
	35	1.0461	1.0374	1.0286	1.0201	1.0116	1.0032	0.9947	0.9866	0.9779
	40	1.0488	1.0403	1.0316	1.0232	1.0148	1.0065	0.9983	0.9903	0.9817
	45	1.0515	1.0431	1.0345	1.0263	1.0179	1.0099	1.0017	0.9937	0.9854
	50	1.0541	1.0457	1.0374	1.0291	1.0210	1.0129	1.0050	0.9972	0.9890
	55	1.0567	1.0485	1.0401	1.0321	1.0241	1.0162	1.0083	1.0006	0.9926
	60	1.0593	1.0510	1.0430						
0.2896	10	1.0563	1.0460	1.0357						
	15	1.0598	1.0497	1.0396						
	20	1.0632	1.0533	1.0434						
	25	1.0665	1.0568	1.0470						
	30	1.0697	1.0601	1.0506						
	35	1.0728	1.0634	1.0540						
	40	1.0759	1.0666	1.0573						
	45	1.0788	1.0697	1.0606						
	50	1.0818	1.0727	1.0637						
	55	1.0846	1.0757	1.0668	1.0581	1.0495	1.0410	1.0325	1.0241	1.0157
	60	1.0874	1.0785	1.0699	1.0613	1.0528	1.0443	1.0359	1.0277	1.0194

These data are considered here. The complete data set is very extensive. Only this portion is used in the example, here.

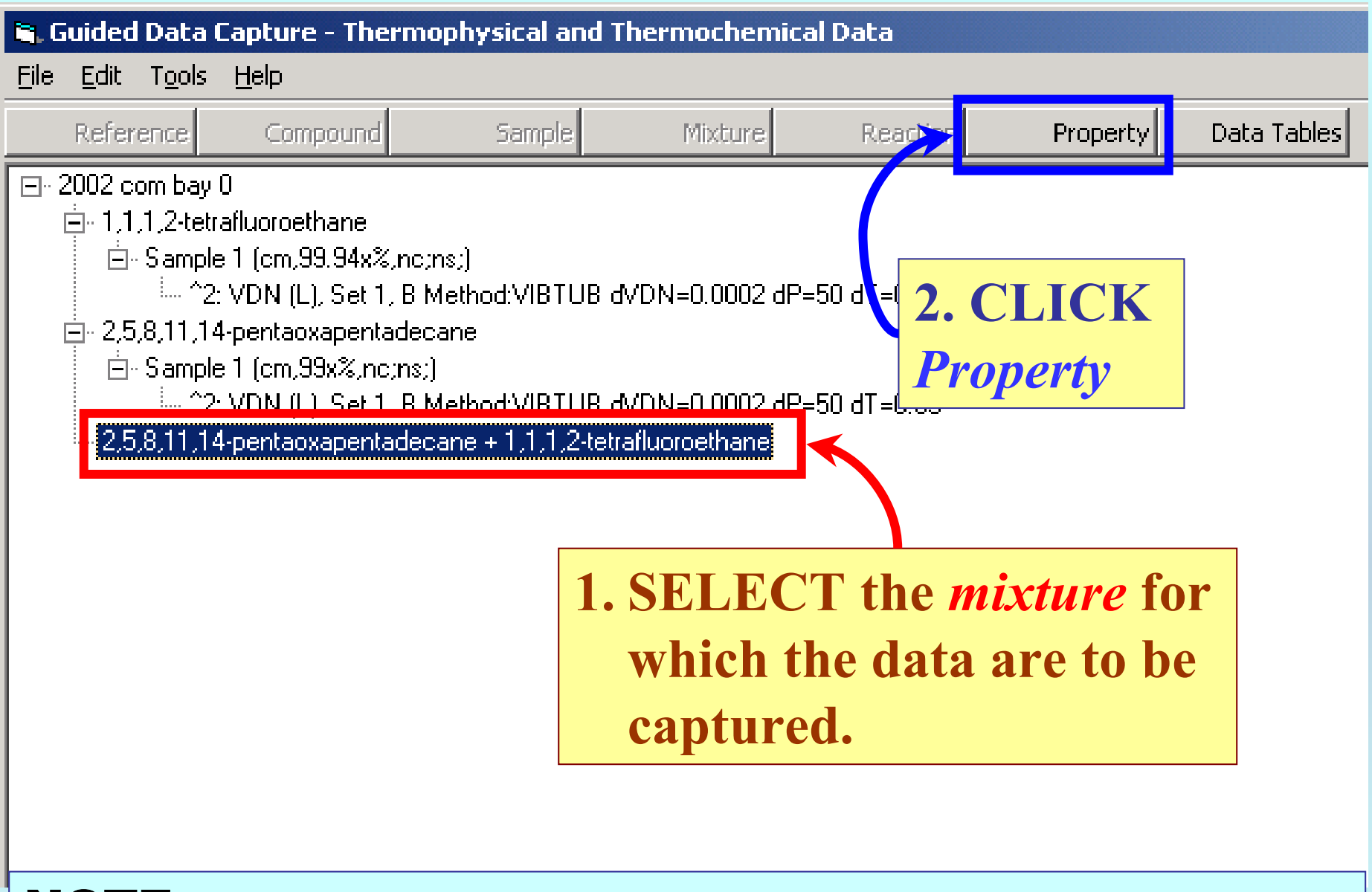
Experimental Method Info:

Vibrating-tube densimeter

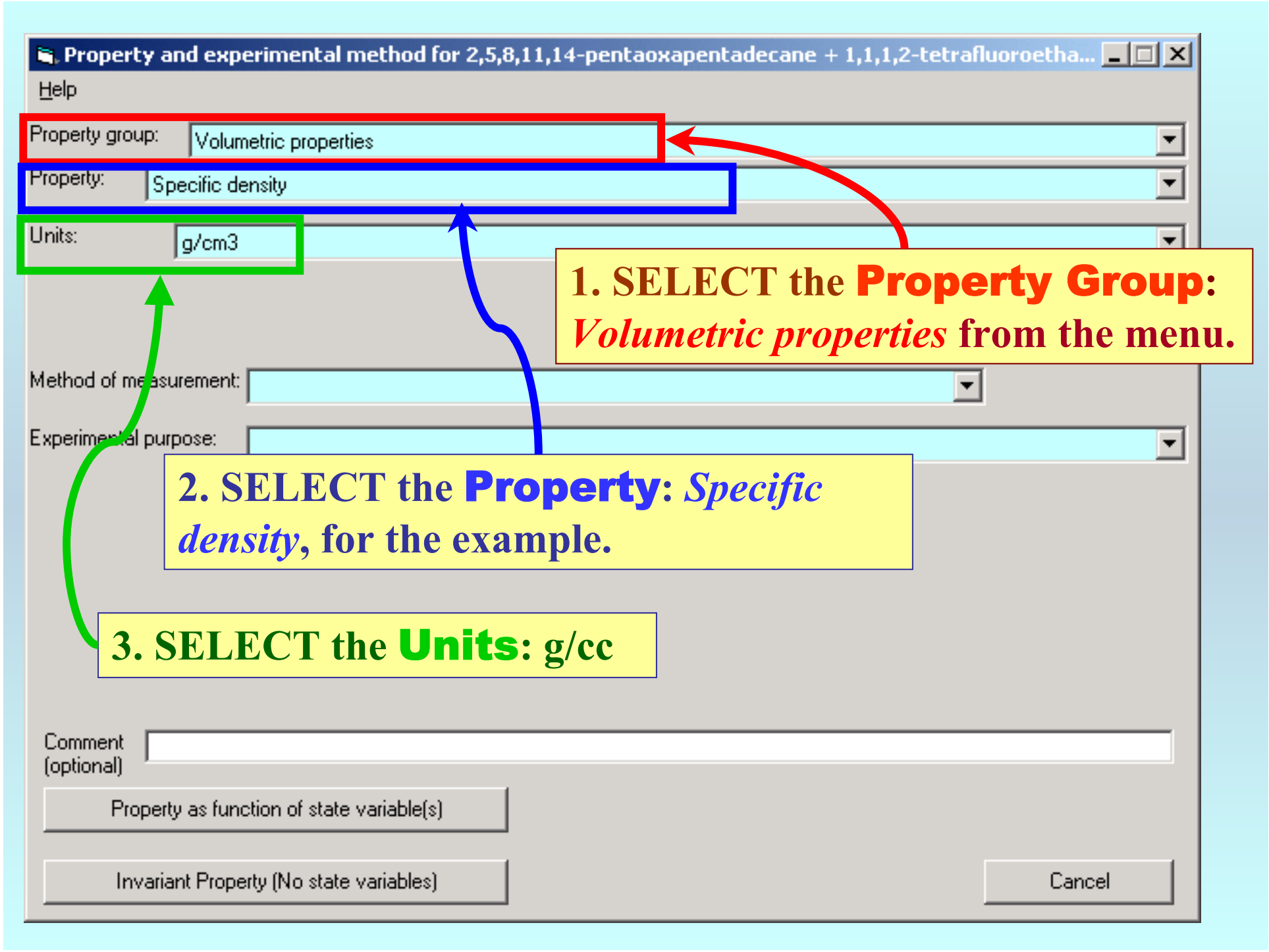
Uncertainty in density = 0.0002 g/cc

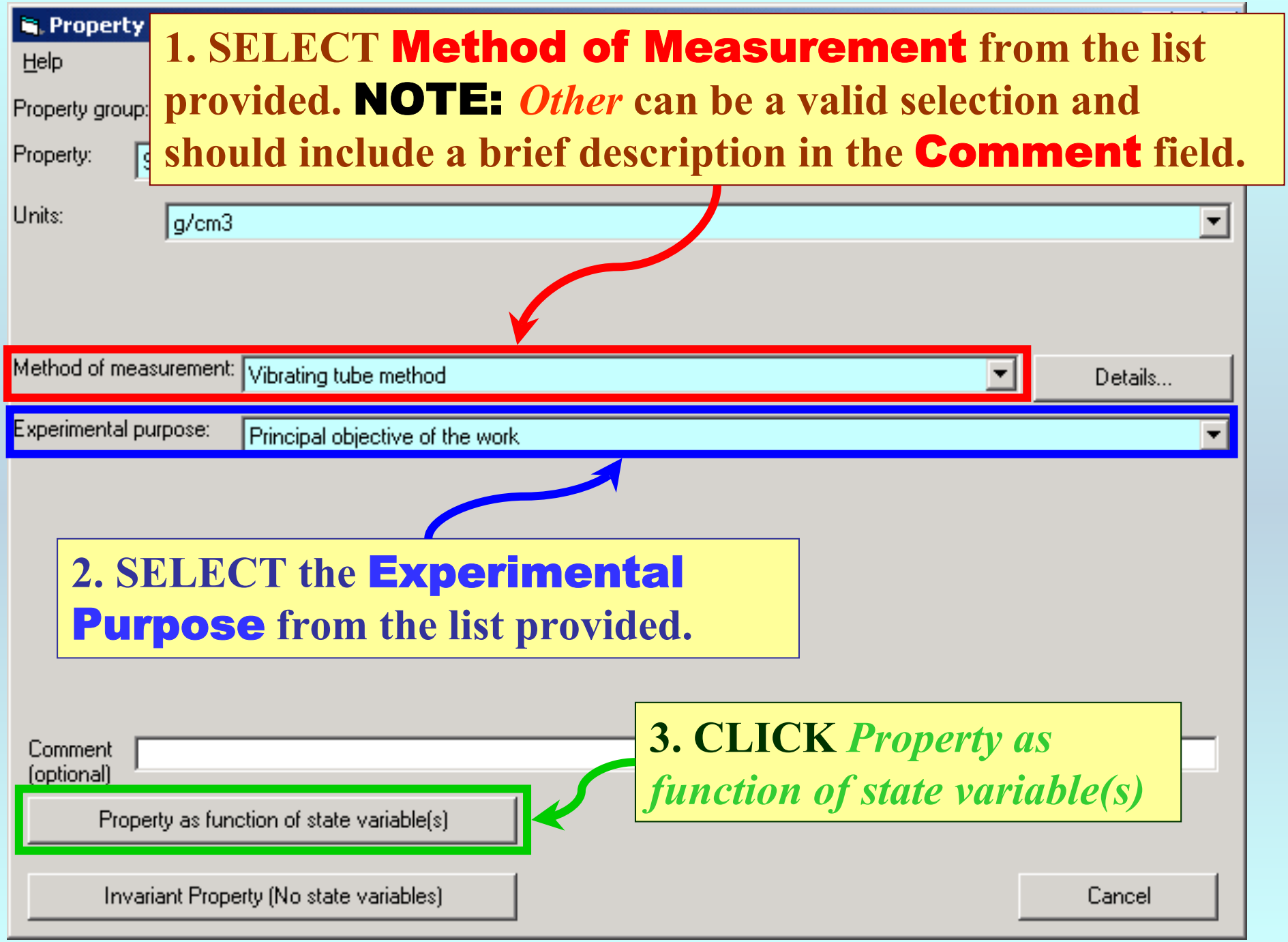
Uncertainty in temperature = 0.05 K

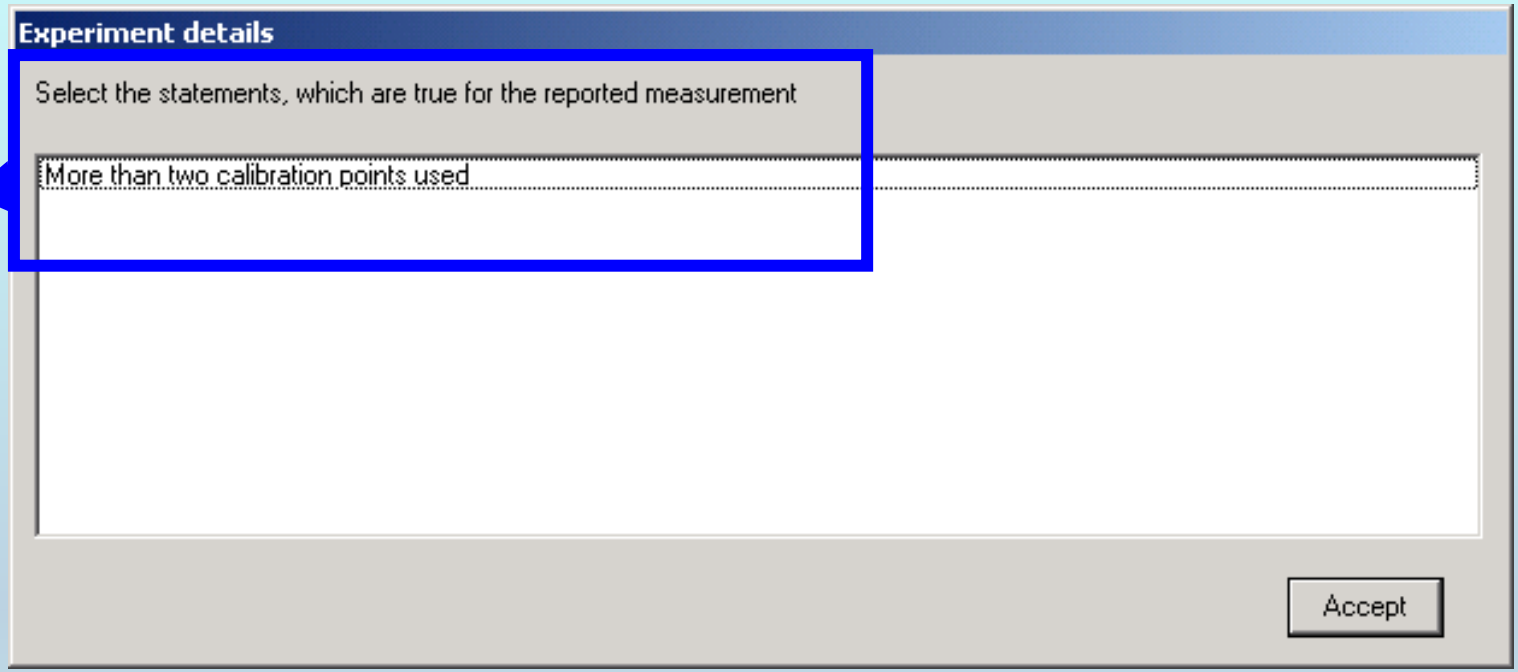
Uncertainty in pressure = 0.05 MPa



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.)

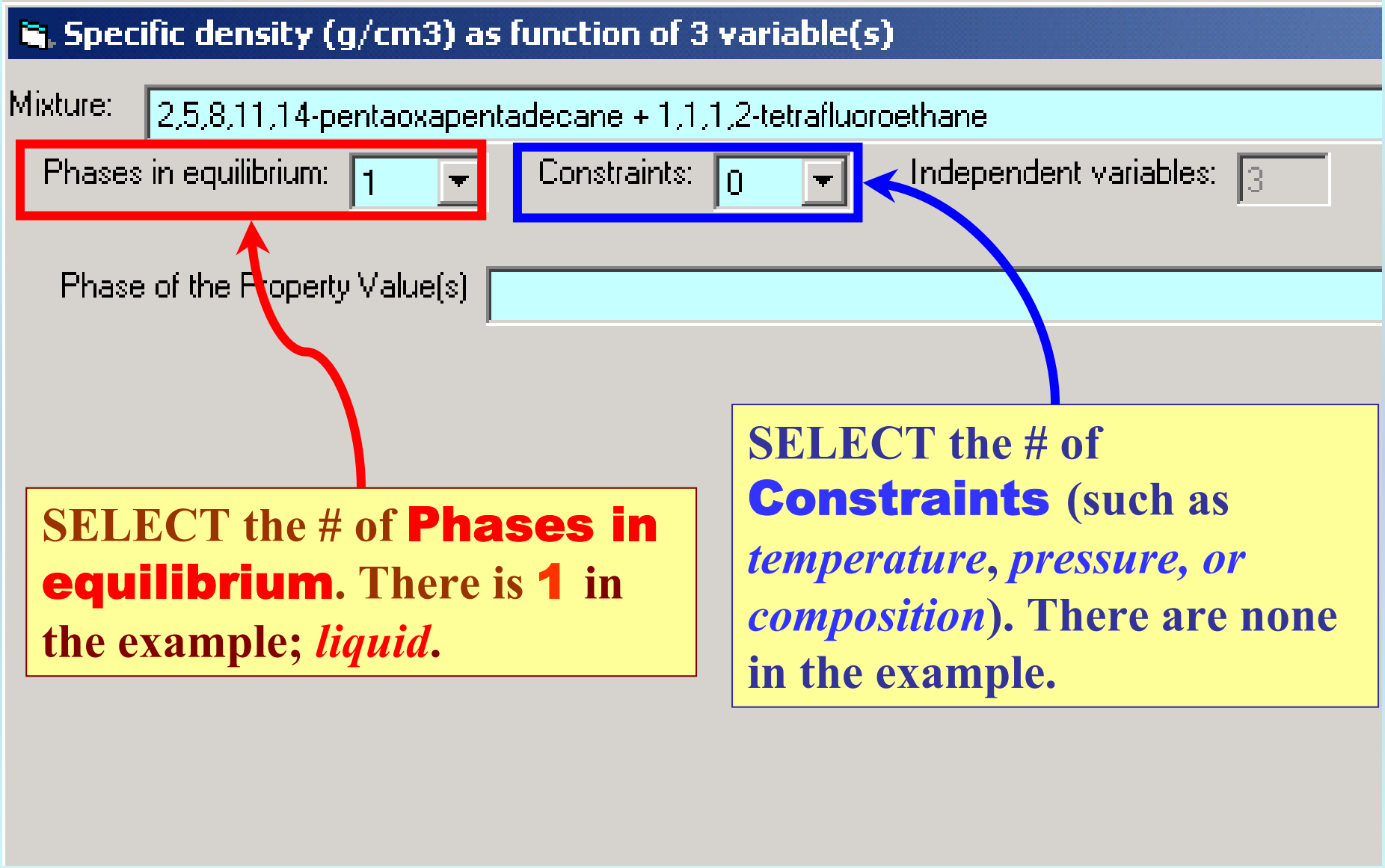

Property and experimental method for 2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroetha...
Help
Property group:
Volumetric properties
Property:
Specific density
Units:
g/cm3
1. SELECT the Property Group: Volumetric properties from the menu.
Method of measurement:
Experimental purpose:
2. SELECT the Property: Specific density, for the example.
3. SELECT the Units: g/cc
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
Cancel


Property
Help
Property group:
Property:
Units:
g/cm3
Method of measurement:
Vibrating tube method
Details...
Experimental purpose:
Principal objective of the work
Comment (optional)
Property as function of state variable(s)
Invariant Property (No state variables)
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 Property as function of state variable(s)



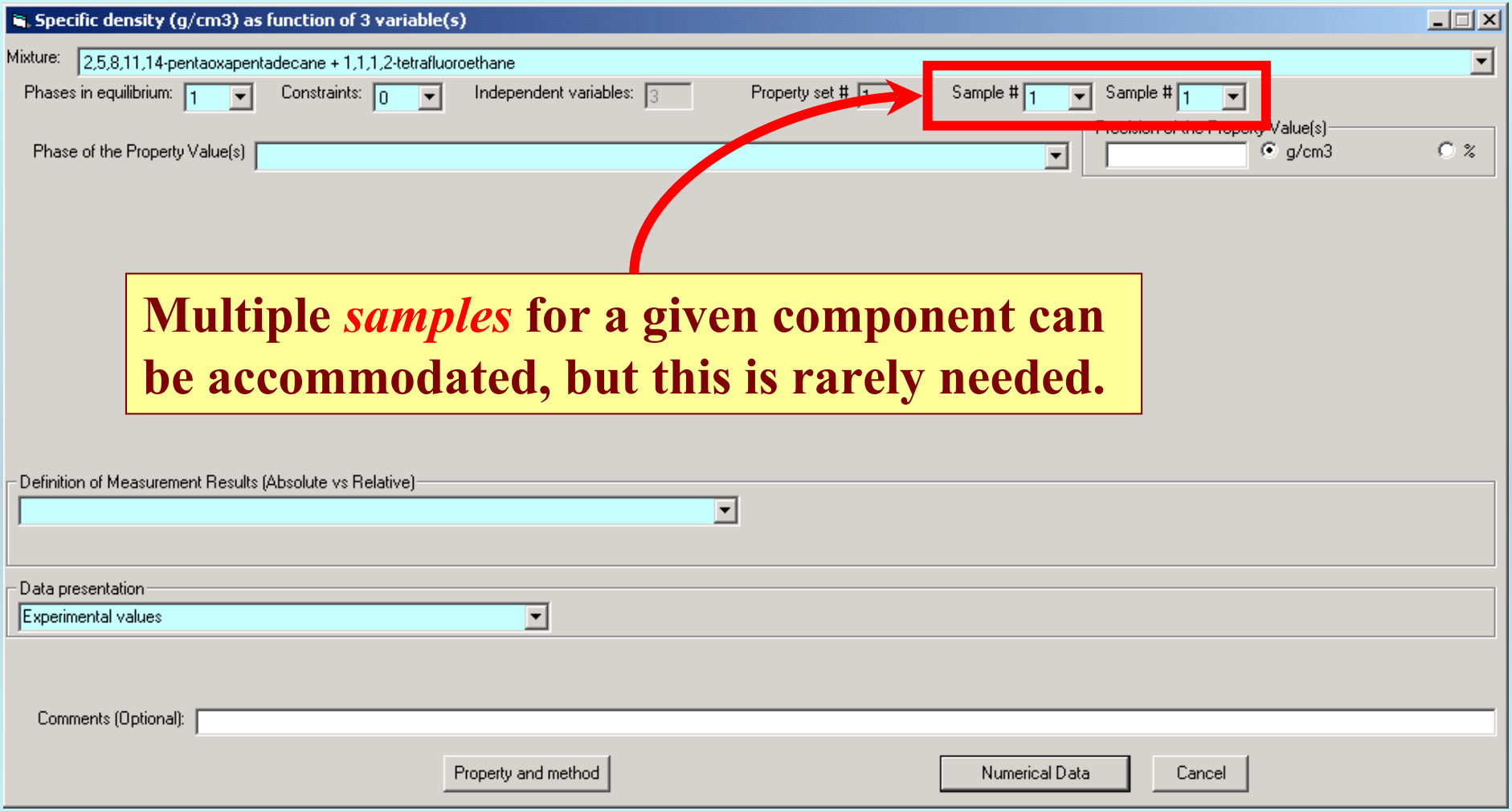
NOTE: For some methods, additional information is requested.

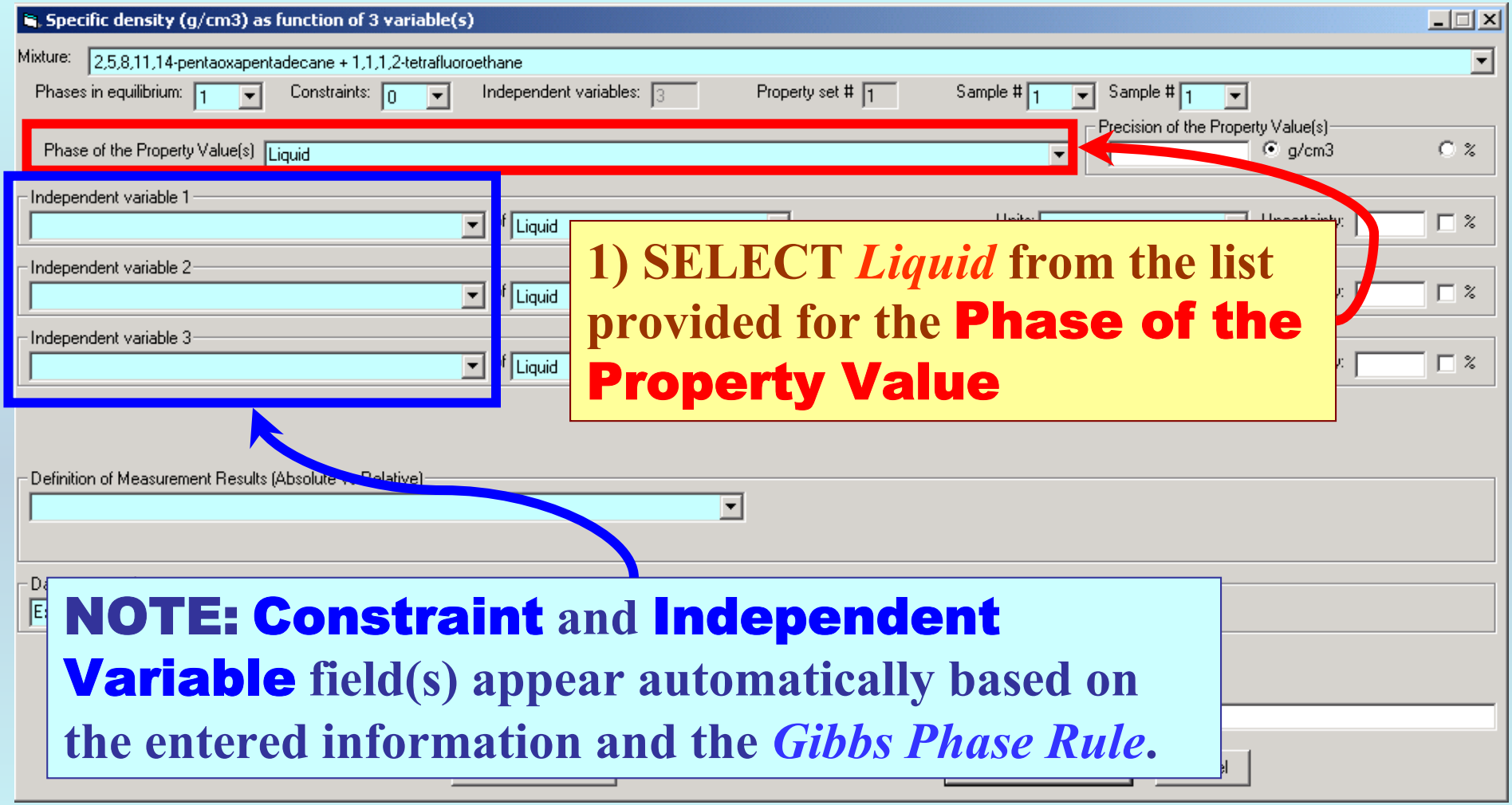
SELECTION of # of Phases in Equilibrium and # of Constraints



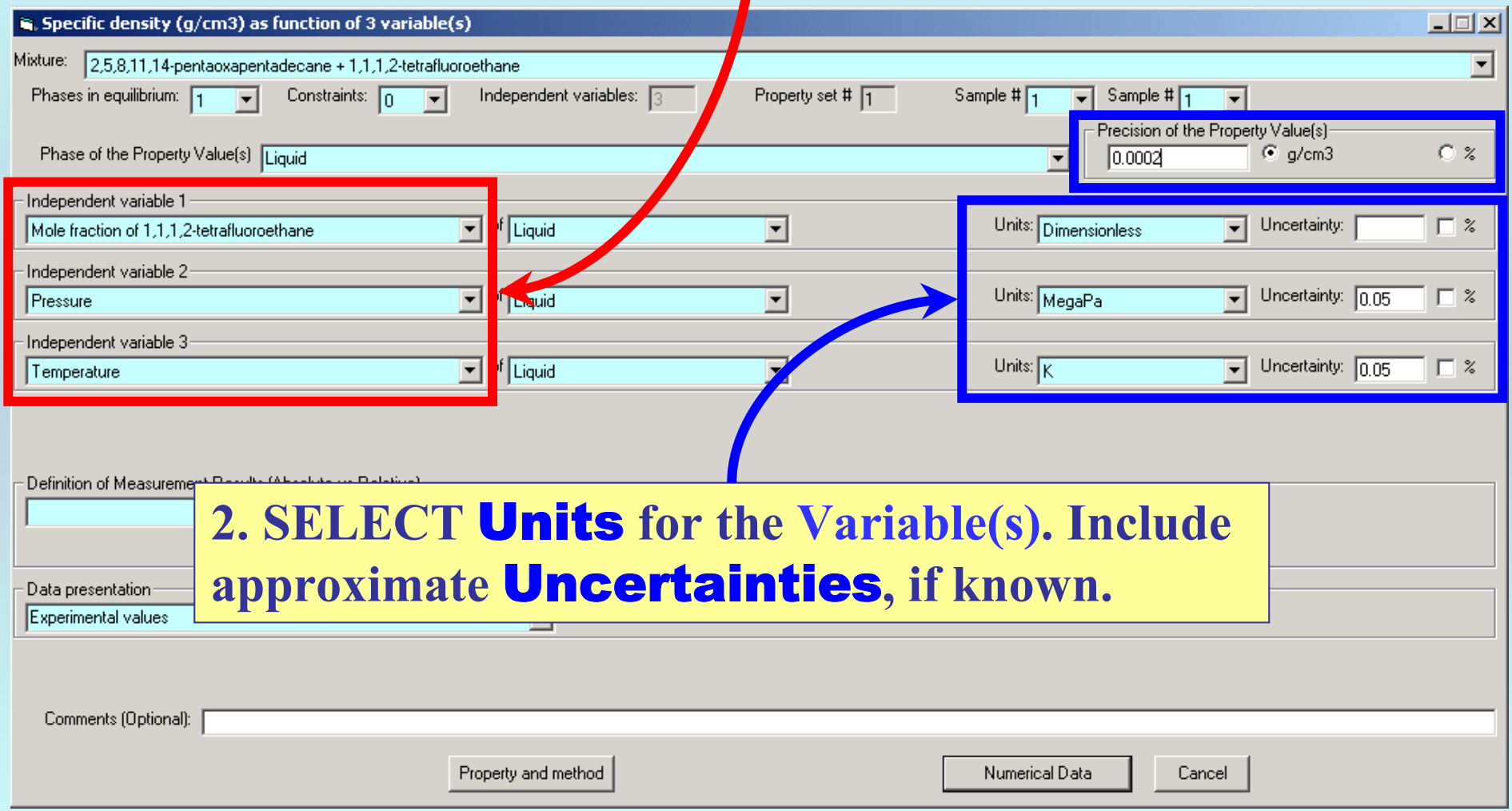
SELECT the # of **Phases in equilibrium**. There is **1** in the example; *liquid*.

SELECT the # of **Constraints** (such as *temperature*, *pressure, or composition*). There are none in the example.

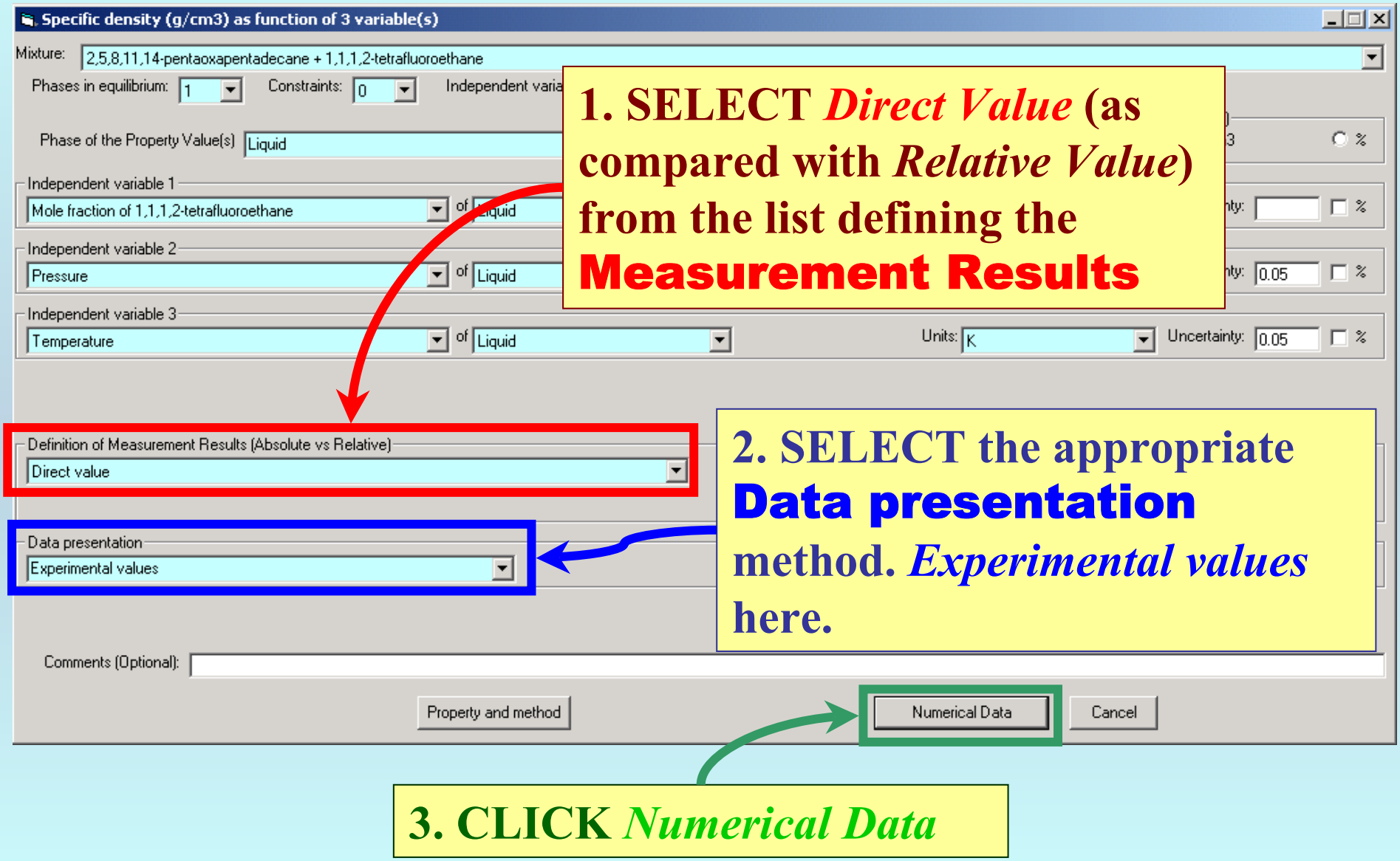

Specific density (g/cm3) as function of 3 variable(s)
Mixture:
2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroethane
Phases in equilibrium:
1
Constraints:
0
Independent variables:
3
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
g/cm3
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel

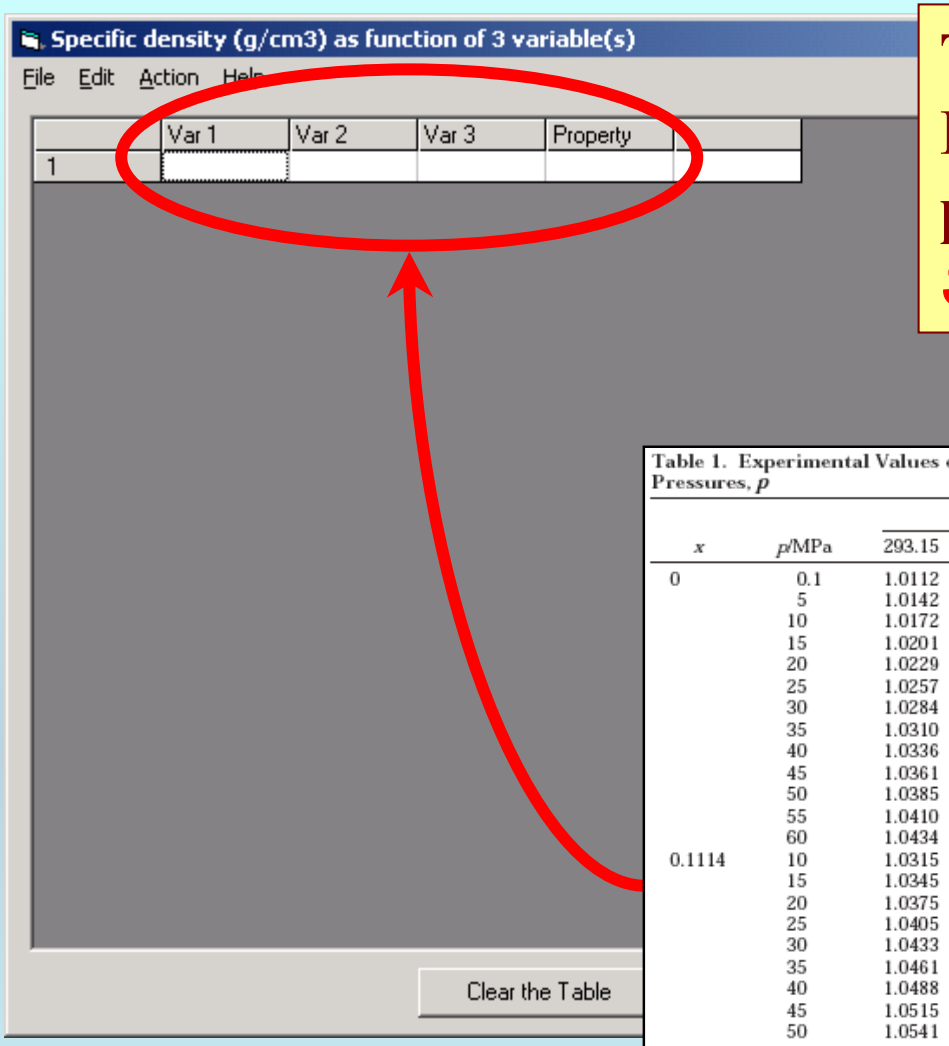

Specific density (g/cm3) as function of 3 variable(s)
Mixture:
2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroethane
Phases in equilibrium:
1
Constraints:
0
Independent variables:
3
Property set #
1
Sample #
1
Sample #
1
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
g/cm3
%
Independent variable 1
Independent variable 2
Independent variable 3
Liquid
Liquid
Liquid
Definition of Measurement Results (Absolute
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 entered information and the Gibbs Phase Rule.

1. SELECT the **Independent Variable(s)** from the menus.



2. SELECT **Units** for the Variable(s). Include approximate **Uncertainties**, if known.


Specific density (g/cm3) as function of 3 variable(s)
Mixture: 2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroethane
Phases in equilibrium: 1
Constraints: 0
Phase of the Property Value(s): Liquid
Independent variable 1
Mole fraction of 1,1,1,2-tetrafluoroethane
of Liquid
Independent variable 2
Pressure
of Liquid
Independent variable 3
Temperature
of Liquid
Units: K
Uncertainty: 0.05
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Comments (Optional):
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...

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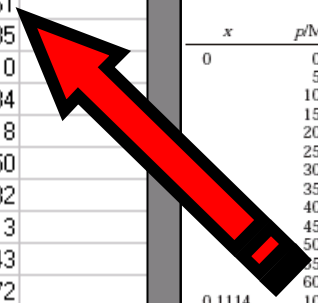
0	0.1	1.0112	1.0018	0.9925	0.9833	0.9740	0.9648	0.9556	0.9469	0.9375
	5	1.0142	1.0050	0.9959	0.9868	0.9778	0.9687	0.9598	0.9513	0.9423
	10	1.0172	1.0082	0.9992	0.9903	0.9814	0.9726	0.9639	0.9557	0.9468
	15	1.0201	1.0113	1.0025	0.9937	0.9850	0.9764	0.9679	0.9598	0.9511
	20	1.0229	1.0143	1.0055	0.9970	0.9883	0.9800	0.9716	0.9639	0.9552
	25	1.0257	1.0172	1.0086	1.0001	0.9917	0.9835	0.9752	0.9675	0.9593
	30	1.0284	1.0200	1.0116	1.0032	0.9950	0.9869	0.9788	0.9712	0.9631
	35	1.0310	1.0227	1.0144	1.0063	0.9982	0.9901	0.9821	0.9748	0.9669
	40	1.0336	1.0254	1.0172	1.0091	1.0012	0.9932	0.9855	0.9783	0.9704
	45	1.0361	1.0281	1.0201	1.0121	1.0042	0.9963	0.9886	0.9815	0.9739
	50	1.0385	1.0306	1.0226	1.0147	1.0070	0.9993	0.9917	0.9846	0.9771
	55	1.0410	1.0332	1.0252	1.0175	1.0098	1.0023	0.9947	0.9880	0.9805
	60	1.0434	1.0355	1.0278	1.0202	1.0126	1.0050	0.9976	0.9910	0.9838
0.1114	10	1.0315	1.0220	1.0124	1.0031	0.9936	0.9844	0.9752	0.9659	0.9564
	15	1.0345	1.0254	1.0159	1.0067	0.9975	0.9887	0.9794	0.9704	0.9611
	20	1.0375	1.0285	1.0192	1.0103	1.0011	0.9925	0.9834	0.9746	0.9657
	25	1.0405	1.0316	1.0223	1.0136	1.0047	0.9962	0.9872	0.9787	0.9699
	30	1.0433	1.0346	1.0255	1.0169	1.0081	0.9998	0.9911	0.9828	0.9742
	35	1.0461	1.0374	1.0286	1.0201	1.0116	1.0032	0.9947	0.9866	0.9779
	40	1.0488	1.0403	1.0316	1.0232	1.0148	1.0065	0.9983	0.9903	0.9817
	45	1.0515	1.0431	1.0345	1.0263	1.0179	1.0099	1.0017	0.9937	0.9854
	50	1.0541	1.0457	1.0374	1.0291	1.0210	1.0129	1.0050	0.9972	0.9890
	55	1.0567	1.0485	1.0401	1.0321	1.0241	1.0162	1.0083	1.0006	0.9926
	60	1.0593	1.0510	1.0430	1.0349	1.0269	1.0192	1.0114	1.0038	0.9955
0.2896	10	1.0563	1.0460	1.0357	1.0255	1.0151	1.0050	0.9948	0.9847	0.9742
	15	1.0598	1.0497	1.0396	1.0296	1.0196	1.0097	0.9997	0.9899	0.9798
	20	1.0632	1.0533	1.0434	1.0337	1.0237	1.0142	1.0044	0.9948	0.9850
	25	1.0665	1.0568	1.0470	1.0375	1.0278	1.0185	1.0089	0.9995	0.9899
	30	1.0697	1.0601	1.0506	1.0412	1.0317	1.0225	1.0132	1.0039	0.9947
	35	1.0728	1.0634	1.0540	1.0447	1.0355	1.0265	1.0173	1.0083	0.9991
	40	1.0759	1.0666	1.0573	1.0482	1.0392	1.0303	1.0213	1.0125	1.0035
	45	1.0788	1.0697	1.0606	1.0517	1.0428	1.0339	1.0250	1.0164	1.0076
	50	1.0818	1.0727	1.0637	1.0548	1.0461	1.0374	1.0287	1.0203	1.0116
	55	1.0846	1.0757	1.0668	1.0581	1.0495	1.0410	1.0325	1.0241	1.0157
	60	1.0874	1.0785	1.0699	1.0613	1.0528	1.0443	1.0359	1.0277	1.0194

Specific density (g/cm3) as function of 3 variable(s)

File Edit Action Help

	Var 1	Var 2	Var 3	Property
1	0	0.1	293.15	1.0112
2	0	5	293.15	1.0142
3	0	10	293.15	1.0172
4	0	15	293.15	1.0201
5	0	20	293.15	1.0229
6	0	25	293.15	1.0257
7	0	30	293.15	1.0284
8	0	35	293.15	1.0310
9	0	40	293.15	1.0336
10	0	45	293.15	1.0361
11	0	50	293.15	1.0385
12	0	55	293.15	1.0410
13	0	60	293.15	1.0434
14	0	0.1	303.15	1.0018
15	0	5	303.15	1.0050
16	0	10	303.15	1.0082
17	0	15	303.15	1.0113
18	0	20	303.15	1.0143
19	0	25	303.15	1.0172
20	0	30	303.15	1.0200
21	0	35	303.15	1.0227
22	0	40	303.15	1.0254
23	0	45	303.15	1.0281
24	0	50	303.15	1.0306
25	0	55	303.15	1.0332

Clear the Table View p



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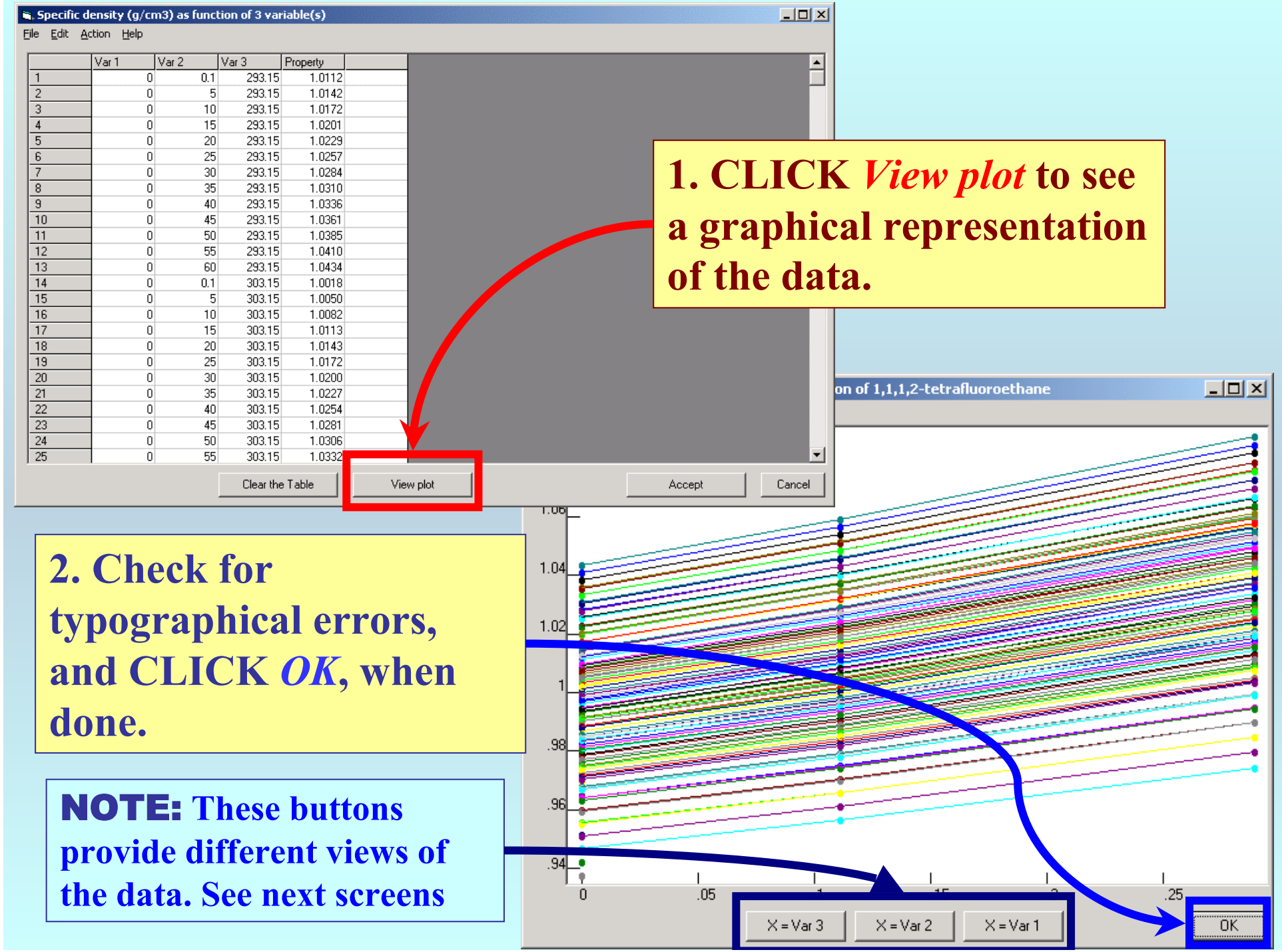
0	0.1	1.0112	1.0018	0.9925	0.9833	0.9740	0.9648	0.9556	0.9469	0.9375
	5	1.0142	1.0050	0.9959	0.9868	0.9778	0.9687	0.9598	0.9513	0.9423
	10	1.0172	1.0082	0.9992	0.9903	0.9814	0.9726	0.9639	0.9557	0.9468
	15	1.0201	1.0113	1.0025	0.9937	0.9850	0.9764	0.9679	0.9598	0.9511
	20	1.0229	1.0143	1.0055	0.9970	0.9883	0.9800	0.9716	0.9639	0.9552
	25	1.0257	1.0172	1.0086	1.0001	0.9917	0.9835	0.9752	0.9675	0.9593
	30	1.0284	1.0200	1.0116	1.0032	0.9950	0.9869	0.9788	0.9712	0.9631
	35	1.0310	1.0227	1.0144	1.0063	0.9982	0.9901	0.9821	0.9748	0.9669
	40	1.0336	1.0254	1.0172	1.0091	1.0012	0.9932	0.9855	0.9783	0.9704
	45	1.0361	1.0281	1.0201	1.0121	1.0042	0.9963	0.9886	0.9815	0.9739
	50	1.0385	1.0306	1.0226	1.0147	1.0070	0.9993	0.9917	0.9846	0.9771
	55	1.0410	1.0332	1.0252	1.0175	1.0098	1.0023	0.9947	0.9880	0.9805
	60	1.0434	1.0355	1.0278	1.0202	1.0126	1.0050	0.9976	0.9910	0.9838
0.1114	10	1.0315	1.0220	1.0124	1.0031	0.9936	0.9844	0.9752	0.9659	0.9564
	15	1.0345	1.0254	1.0159	1.0067	0.9975	0.9887	0.9794	0.9704	0.9611
	20	1.0375	1.0285	1.0192	1.0103	1.0011	0.9925	0.9834	0.9746	0.9657
	25	1.0405	1.0316	1.0223	1.0136	1.0047	0.9962	0.9872	0.9787	0.9699
	30	1.0433	1.0346	1.0255	1.0169	1.0081	0.9998	0.9911	0.9828	0.9742
	35	1.0461	1.0374	1.0286	1.0201	1.0116	1.0032	0.9947	0.9866	0.9779
	40	1.0488	1.0403	1.0316	1.0232	1.0148	1.0065	0.9983	0.9903	0.9817
	45	1.0515	1.0431	1.0345	1.0263	1.0179	1.0099	1.0017	0.9937	0.9854
	50	1.0541	1.0457	1.0374	1.0291	1.0210	1.0129	1.0050	0.9972	0.9890
	55	1.0567	1.0485	1.0401	1.0321	1.0241	1.0162	1.0083	1.0006	0.9926
	60	1.0593	1.0510	1.0430	1.0349	1.0269	1.0192	1.0114	1.0038	0.9955
0.2896	10	1.0563	1.0460	1.0357	1.0255	1.0151	1.0050	0.9948	0.9847	0.9742
	15	1.0598	1.0497	1.0396	1.0296	1.0196	1.0097	0.9997	0.9899	0.9798
	20	1.0632	1.0533	1.0434	1.0337	1.0237	1.0142	1.0044	0.9948	0.9850
	25	1.0665	1.0568	1.0470	1.0375	1.0278	1.0185	1.0089	0.9995	0.9899
	30	1.0697	1.0601	1.0506	1.0412	1.0317	1.0225	1.0132	1.0039	0.9947
	35	1.0728	1.0634	1.0540	1.0447	1.0355	1.0265	1.0173	1.0083	0.9991
	40	1.0759	1.0666	1.0573	1.0482	1.0392	1.0303	1.0213	1.0125	1.0035
	45	1.0788	1.0697	1.0606	1.0517	1.0428	1.0339	1.0250	1.0164	1.0076
	50	1.0818	1.0727	1.0637	1.0548	1.0461	1.0374	1.0287	1.0203	1.0116
	55	1.0846	1.0757	1.0668	1.0581	1.0495	1.0410	1.0325	1.0241	1.0157
	60	1.0874	1.0785	1.0699	1.0613	1.0528	1.0443	1.0359	1.0277	1.0194

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.)


Specific density (g/cm3) as function of 3 variable(s)
File Edit Action Help
Var 1 Var 2 Var 3 Property
1 0 0.1 293.15 1.0112
2 0 5 293.15 1.0142
3 0 10 293.15 1.0172
4 0 15 293.15 1.0201
5 0 20 293.15 1.0229
6 0 25 293.15 1.0257
7 0 30 293.15 1.0284
8 0 35 293.15 1.0310
9 0 40 293.15 1.0336
10 0 45 293.15 1.0361
11 0 50 293.15 1.0385
12 0 55 293.15 1.0410
13 0 60 293.15 1.0434
14 0 0.1 303.15 1.0018
15 0 5 303.15 1.0050
16 0 10 303.15 1.0082
17 0 15 303.15 1.0113
18 0 20 303.15 1.0143
19 0 25 303.15 1.0172
20 0 30 303.15 1.0200
21 0 35 303.15 1.0227
22 0 40 303.15 1.0254
23 0 45 303.15 1.0281
24 0 50 303.15 1.0306
25 0 55 303.15 1.0332
Clear the Table
View plot
Accept
Cancel
1. CLICK View plot to see a graphical representation of the data.
on of 1,1,1,2-tetrafluoroethane
1.04
1.02
1
.98
.96
.94
0
.05
.25
X = Var 3
X = Var 2
X = Var 1
OK
2. Check for typographical errors, and CLICK OK, when done.
NOTE: These buttons provide different views of the data. See next screens

Specific density (g/cm3) as function of 3 variable(s)

File Edit Action Help

	Var 1	Var 2	Var 3	Property
1	0	0.1	293.15	1.0112
2	0	5	293.15	1.0142
3	0	10	293.15	1.0172
4	0	15	293.15	1.0201
5	0	20	293.15	1.0229
6	0	25	293.15	1.0257
7	0	30	293.15	1.0284
8	0	35	293.15	1.0310
9	0	40	293.15	1.0336
10	0	45	293.15	1.0361
11	0	50	293.15	1.0385
12	0	55	293.15	1.0410
13	0	60	293.15	1.0434
14	0	0.1	303.15	1.0018
15	0	5	303.15	1.0050
16	0	10	303.15	1.0082
17	0	15	303.15	1.0113
18	0	20	303.15	1.0143
19	0	25	303.15	1.0172
20	0	30	303.15	1.0200
21	0	35	303.15	1.0227
22	0	40	303.15	1.0254
23	0	45	303.15	1.0281
24	0	50	303.15	1.0306
25	0	55	303.15	1.0332

Clear the Table | View plot

NOTE: See **HELP** for addition graph commands.

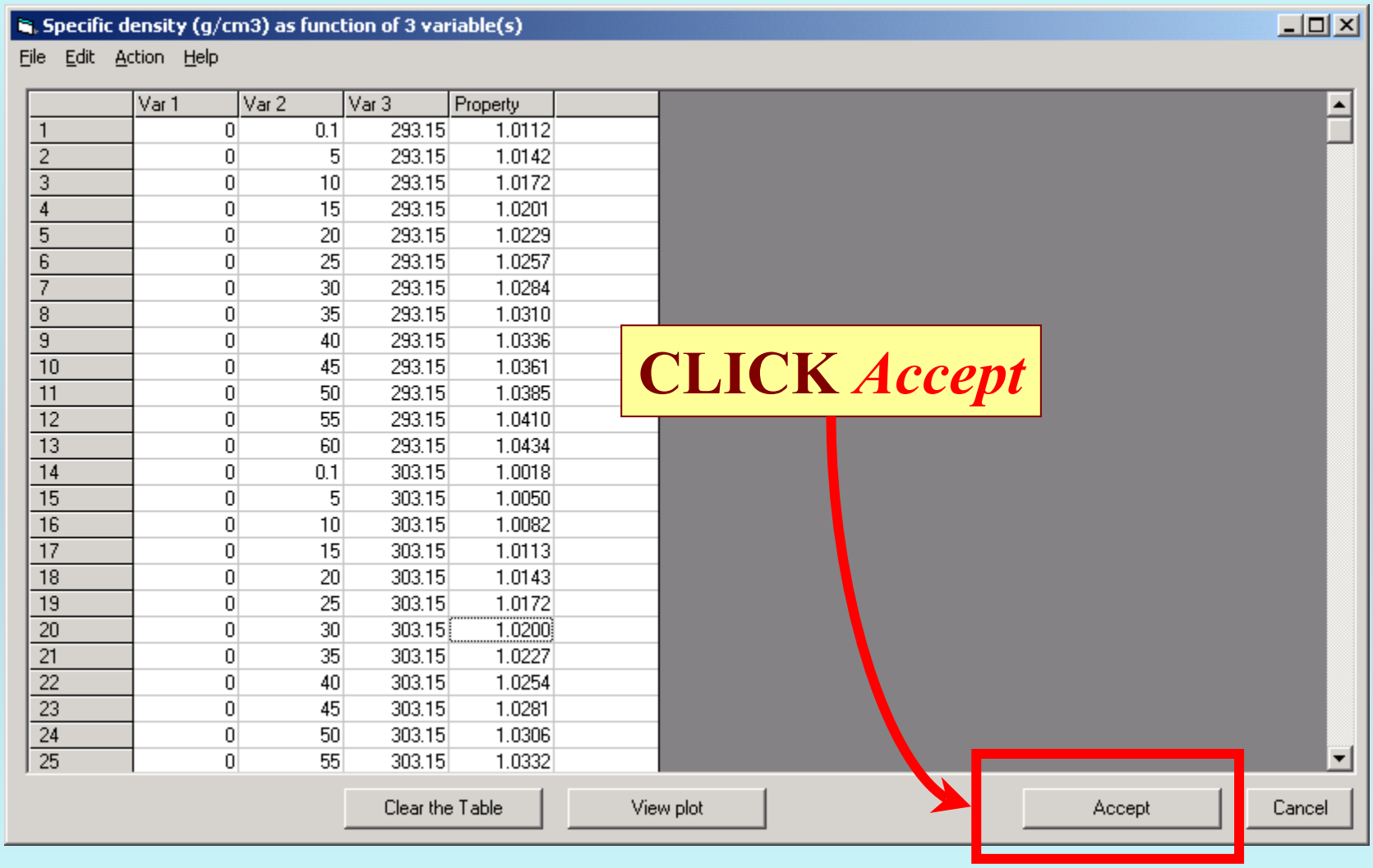
Tools Help

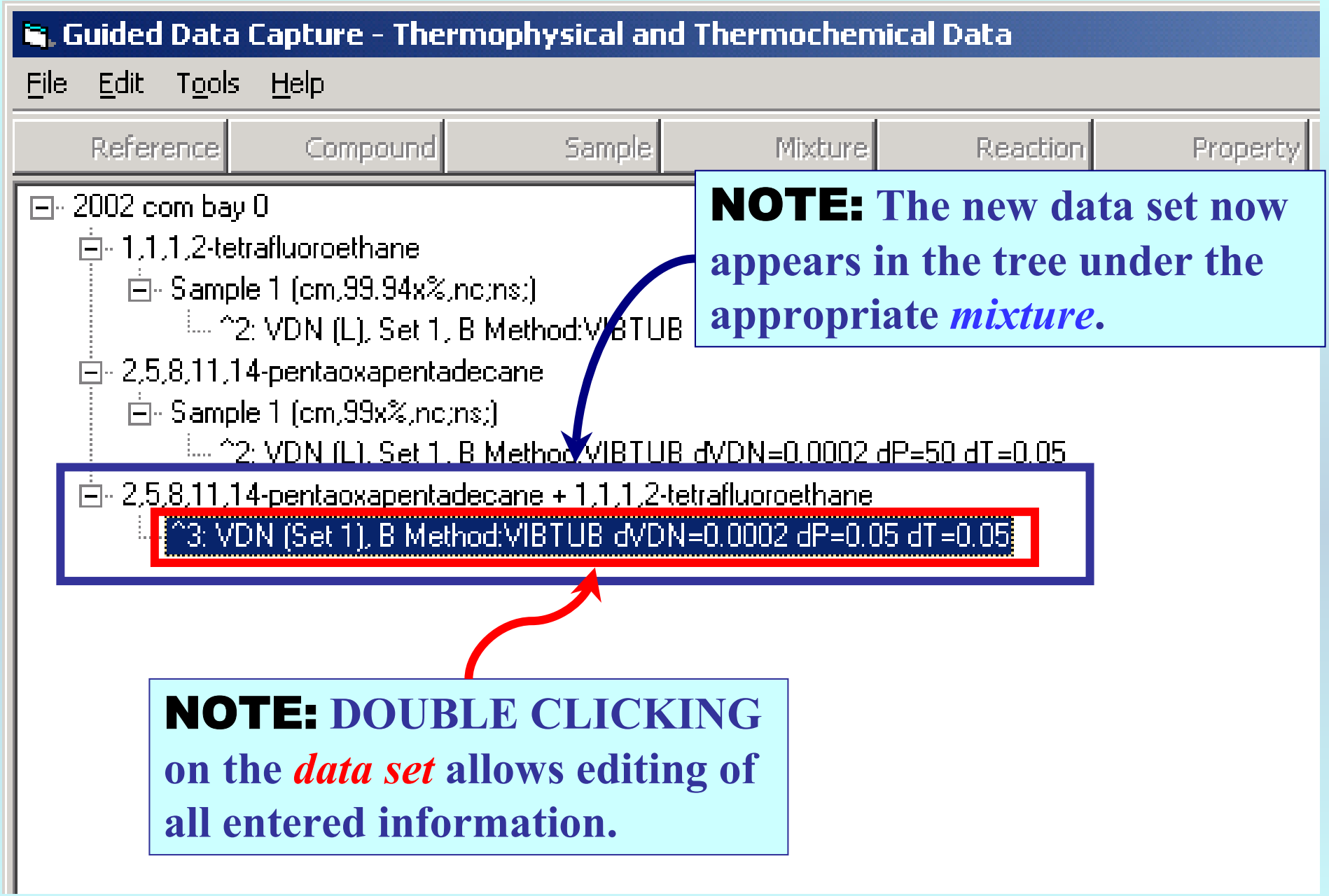
1.035
1.03
1.025
1.02
1.015

0 10 20 30 40 50 60

X = Var 3 | X = Var 2 | X = Var 1 | OK

NOTE: By selecting only part of the data set in the table, clearer views can be obtained.


Specific density (g/cm3) as function of 3 variable(s)
File Edit Action Help
Var 1 Var 2 Var 3 Property
1 0 0.1 293.15 1.0112
2 0 5 293.15 1.0142
3 0 10 293.15 1.0172
4 0 15 293.15 1.0201
5 0 20 293.15 1.0229
6 0 25 293.15 1.0257
7 0 30 293.15 1.0284
8 0 35 293.15 1.0310
9 0 40 293.15 1.0336
10 0 45 293.15 1.0361
11 0 50 293.15 1.0385
12 0 55 293.15 1.0410
13 0 60 293.15 1.0434
14 0 0.1 303.15 1.0018
15 0 5 303.15 1.0050
16 0 10 303.15 1.0082
17 0 15 303.15 1.0113
18 0 20 303.15 1.0143
19 0 25 303.15 1.0172
20 0 30 303.15 1.0200
21 0 35 303.15 1.0227
22 0 40 303.15 1.0254
23 0 45 303.15 1.0281
24 0 50 303.15 1.0306
25 0 55 303.15 1.0332
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction Property
2002 com bay 0
1,1,1,2-tetrafluoroethane
Sample 1 (cm,99.94x%,nc;ns;)
^2: VDN (L), Set 1, B Method:VIBTUB
2,5,8,11,14-pentaoxapentadecane
Sample 1 (cm,99x%,nc;ns;)
^2: VDN (L), Set 1, B Method:VIBTUB dVDN=0.0002 dP=50 dT=0.05
2,5,8,11,14-pentaoxapentadecane + 1,1,1,2-tetrafluoroethane
^3: VDN (Set 1), B Method:VIBTUB dVDN=0.0002 dP=0.05 dT=0.05
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.**