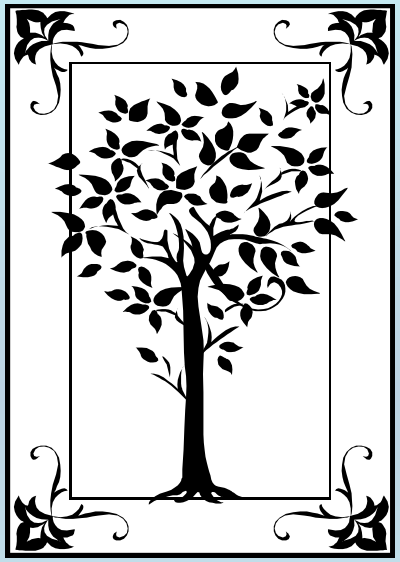
METADATA AND NUMERICAL DATA CAPTURE:
Liquid-Liquid Equilibria
(2-Component: Mutual Solubility / Cloud Point)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **Liquid-Liquid Equilibria (2 components)**
MUTUAL SOLUBILITY / CLOUD POINT
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 1996, *41*, 361−364

Measurement and Correlation of Mutual Solubilities in 2-Butanol + Water

Kenji Ochi,* Tohru Saito, and Kazuo Kojima

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A newly developed laser scattering technique was tested for the determination of mutual solubilities in the 2-butanol + water system at moderate pressures. The liquid−liquid solubility data were measured from the region of solid−liquid equilibria to the upper critical solution temperature. Freezing points in this system were determined by a cooling curve method. A concave curvature of the liquid−liquid line was observed in the vicinity of the freezing points. The solubility data were satisfactorily correlated with Hiranuma's modification of the Wilson equation. The newly measured data compare favorably with previous measurements.

Mutual solubility / Cloud-Point data for **(water + 2-butanol)** at p = 101.3 kPa

Table 1. Experimental Cloud Point Results for 2-Butanol (1) + Water (2)

T/K	x_1[a]	T/K	x_1[a]	T/K	x_1[a]
276.94	0.0738	386.23	0.0965	337.04	0.3279
278.13	0.0725	386.58	0.1050	333.00	0.3307
279.96	0.0705	386.65[b]	0.1151[b]	332.27	0.3312
284.94	0.0642	386.58	0.1219	329.88	0.3321
289.08	0.0590	386.60	0.1318	328.06	0.3330
290.58	0.0571	386.53	0.1417	319.46	0.3330
292.18	0.0553	386.09	0.1524	315.24	0.3312
295.15	0.0522	385.64	0.1599	315.35	0.3307
298.43	0.0491	385.46	0.1686	315.01	0.3314
301.48	0.0471	384.62	0.1796	311.92	0.3279
305.14	0.0452	383.75	0.1900	310.90	0.3279
309.18	0.0421	382.59	0.1985	308.94	0.3277
311.88	0.0406	381.24	0.2094	306.54	0.3253
314.10	0.0393	380.57	0.2181	303.67	0.3229
321.88	0.0371	379.15	0.2267	301.37	0.3191
324.99	0.0361	376.67	0.2365	298.33	0.3150
332.50	0.0342	375.20	0.2434	294.99	0.3088
340.01	0.0342	373.45	0.2503	292.22	0.3019
349.30	0.0361	371.99	0.2580	289.82	0.2947
352.25	0.0371	369.09	0.2668	287.42	0.2891
360.81	0.0393	367.60	0.2708	284.98	0.2823
362.51	0.0406	364.66	0.2791	283.81	0.2762
364.96	0.0421	362.25	0.2857	281.76	0.2692
370.41	0.0459	360.16	0.2914	280.00	0.2667
376.89	0.0530	357.60	0.2981	277.45	0.2636
379.76	0.0573	356.10	0.3003	272.65	0.2667
381.25	0.0621	354.34	0.3036	272.51	0.2692
383.23	0.0680	351.02	0.3104	270.52	0.2726
384.39	0.0751	348.24	0.3150	269.75	0.2726
385.63	0.0820	343.40	0.3211		
386.04	0.0908	339.63	0.3253		

[a] Mole fraction of 2-butanol. [b] The upper critical solution point.

Experimental Method Info:

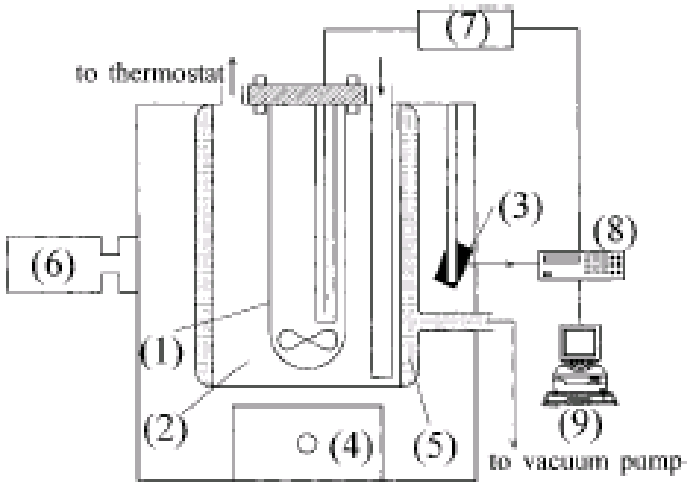
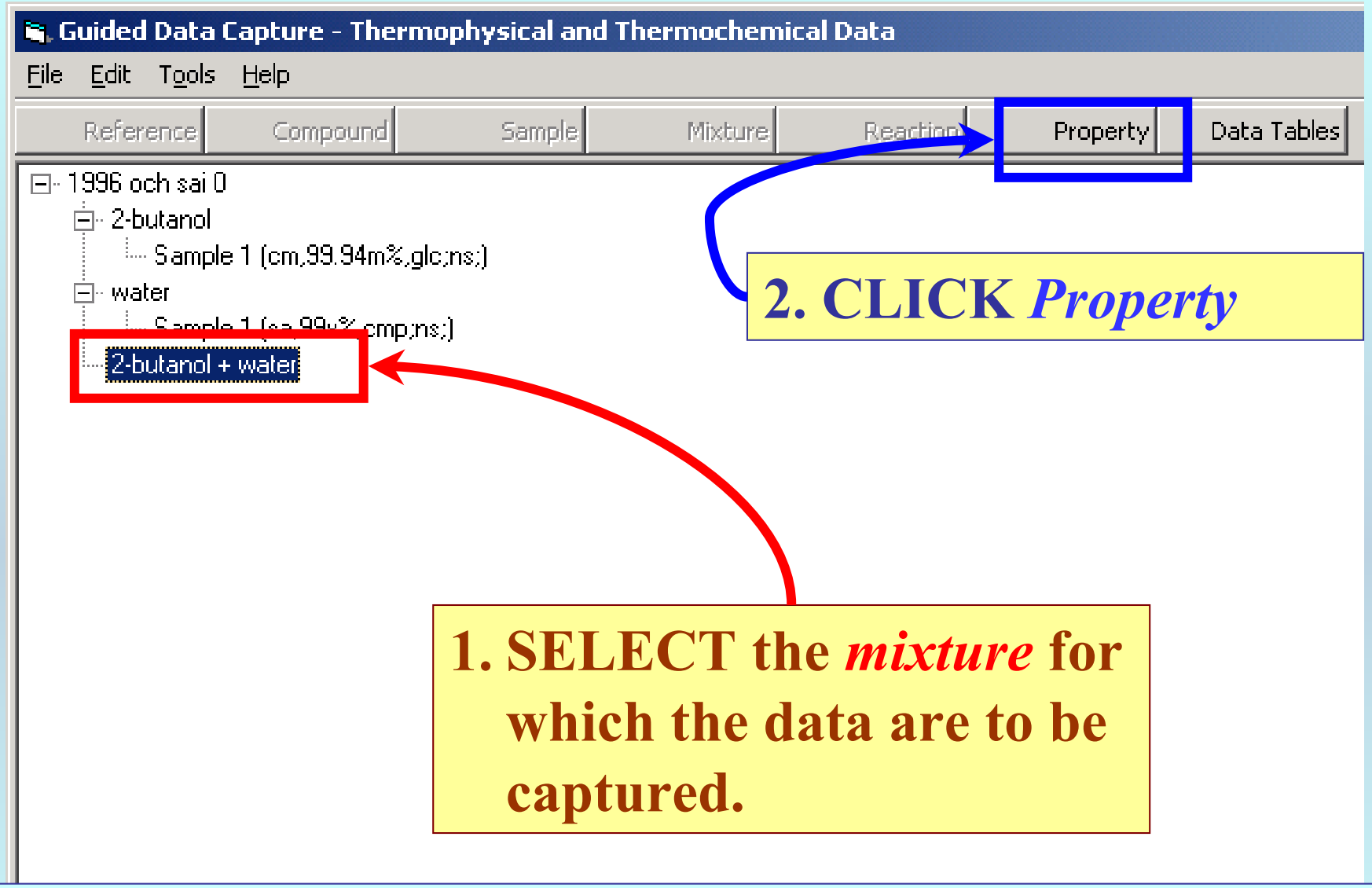
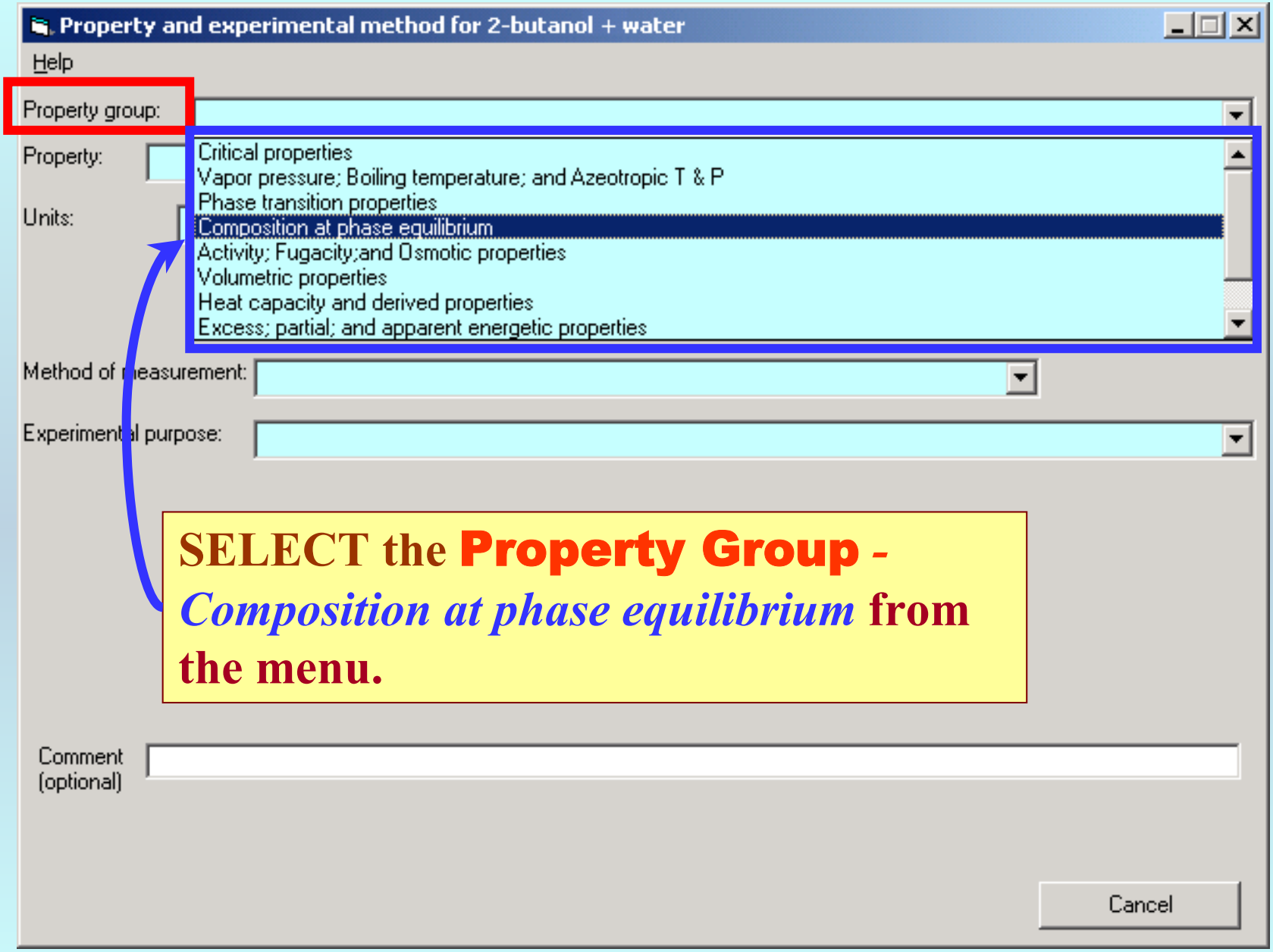


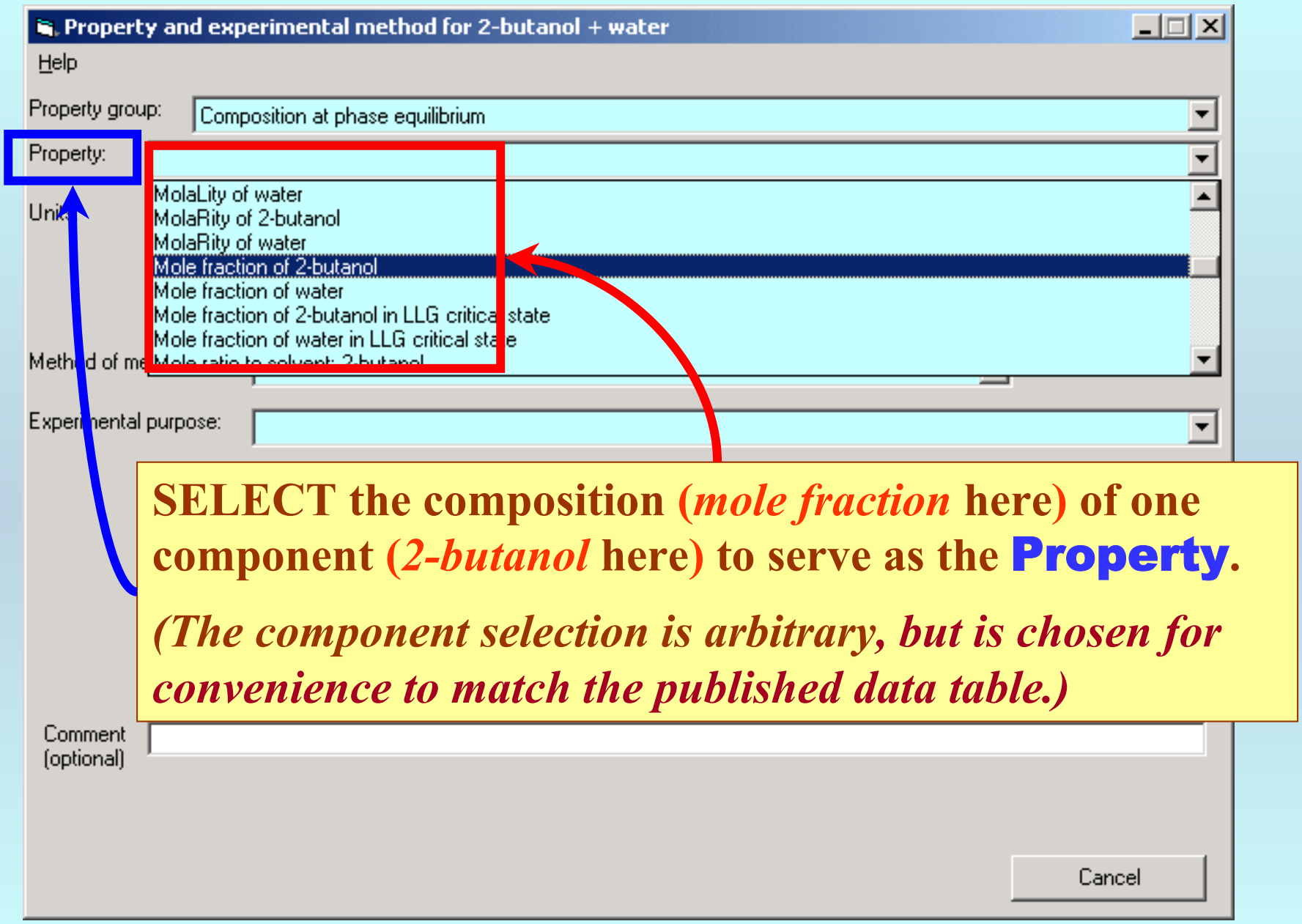
Figure 1. A schematic diagram of the apparatus for measuring the mutual solubility curve: (1) equilibrium cell (pressure glass), (2) temperature bath, (3) light sensor (selenium cell), (4) magnetic stirrer, (5) adiabatic jacket, (6) He−Ne laser, (7) thermometer, (8) digital multimeter, (9) personal computer.

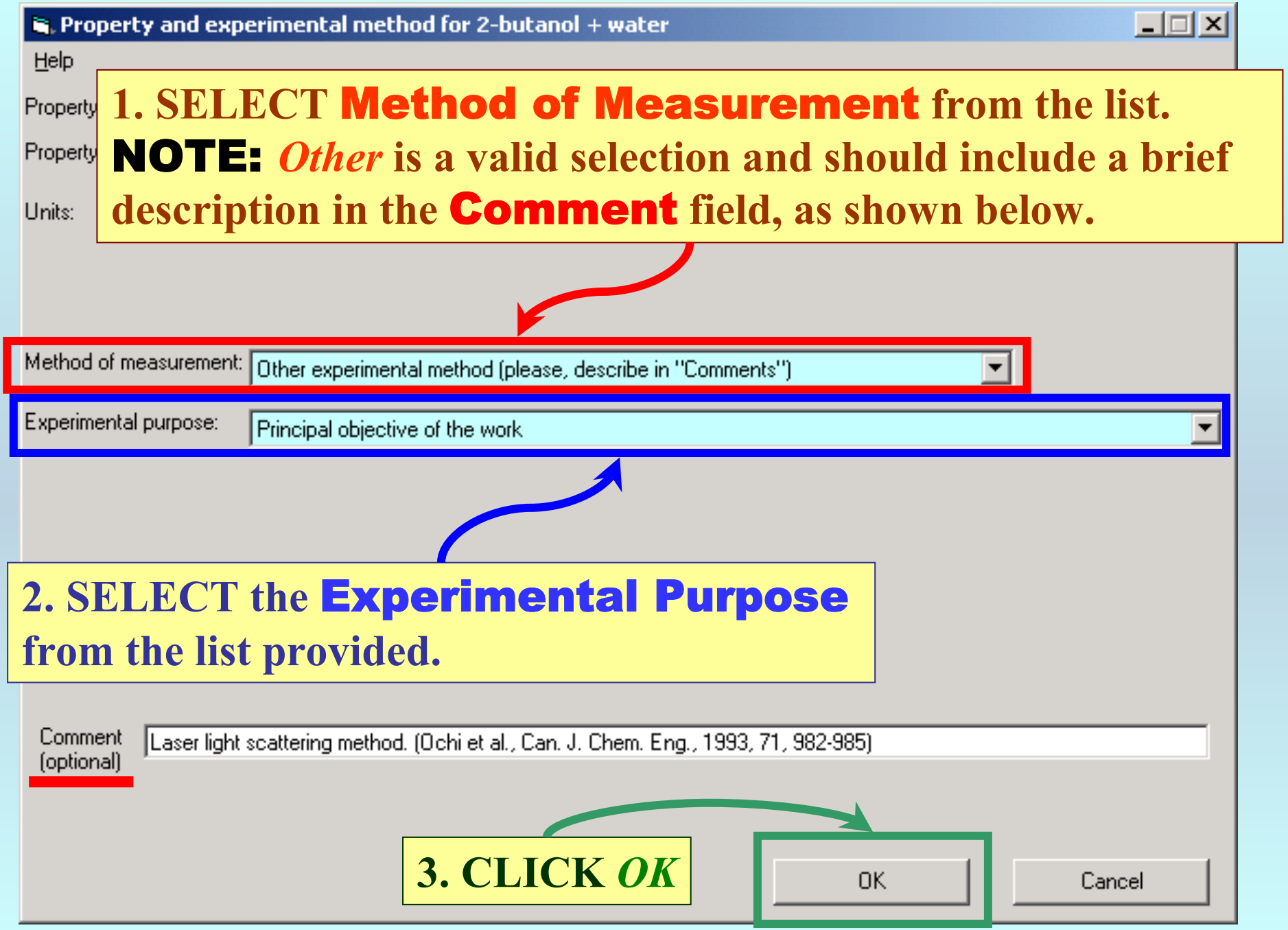
This data set is considered here.



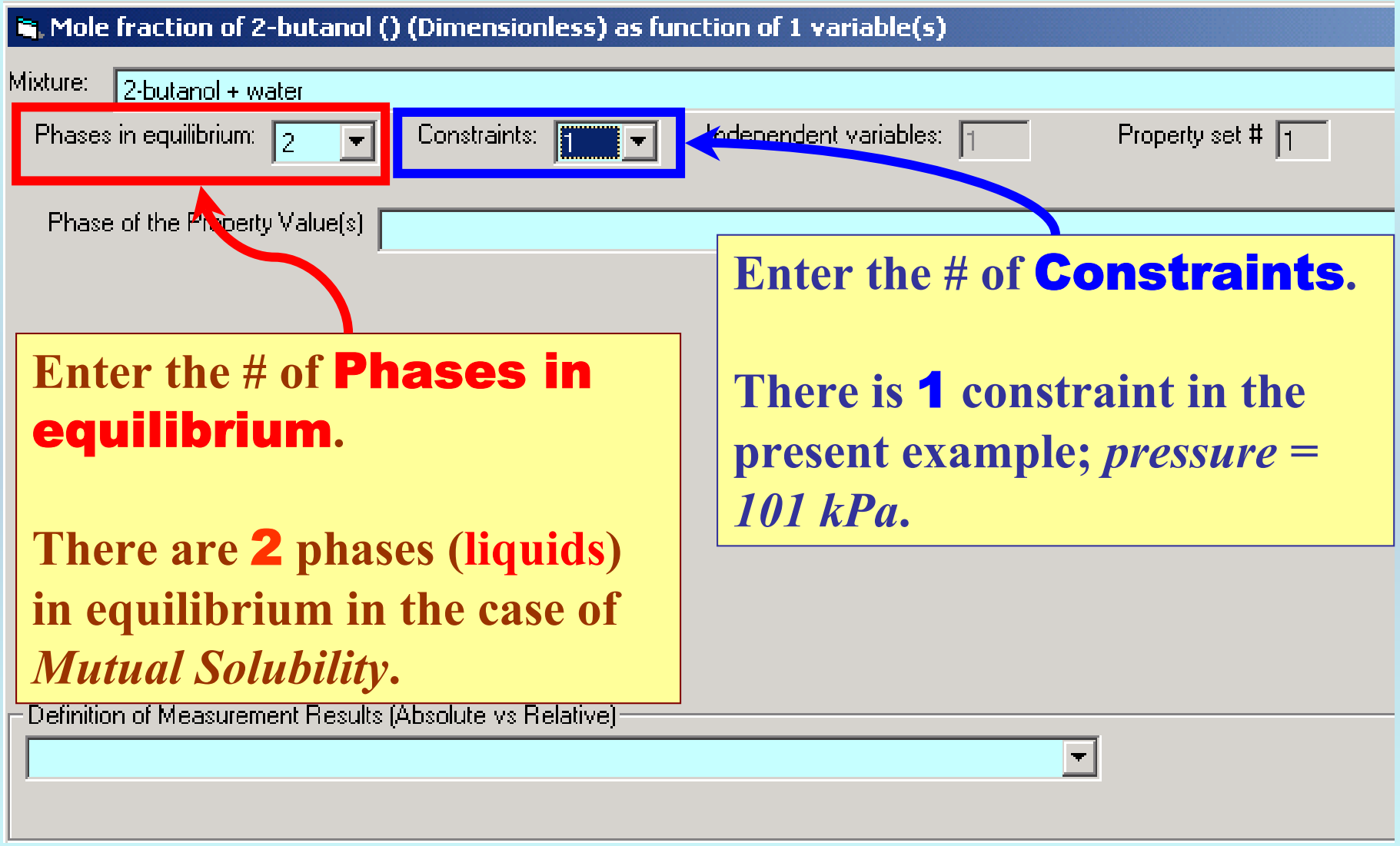
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for 2-butanol + water
Help
Property group:
Property:
Units:
Critical properties
Vapor pressure; Boiling temperature; and Azeotropic T & P
Phase transition properties
Composition at phase equilibrium
Activity; Fugacity;and Osmotic properties
Volumetric properties
Heat capacity and derived properties
Excess; partial; and apparent energetic properties
Method of measurement:
Experimental purpose:
SELECT the Property Group - Composition at phase equilibrium from the menu.
Comment (optional)
Cancel


Property and experimental method for 2-butanol + water
Help
Property group:
Composition at phase equilibrium
Property:
MolaLity of water
MolaRity of 2-butanol
MolaRity of water
Mole fraction of 2-butanol
Mole fraction of water
Mole fraction of 2-butanol in LLG critical state
Mole fraction of water in LLG critical state
Experimental purpose:
SELECT the composition (mole fraction here) of one component (2-butanol here) to serve as the Property.
(The component selection is arbitrary, but is chosen for convenience to match the published data table.)
Comment (optional)
Cancel


Property and experimental method for 2-butanol + water
Help
Property
Property
Units:
1. SELECT Method of Measurement from the list.
NOTE: Other is a valid selection and should include a brief description in the Comment field, as shown below.
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)
Laser light scattering method. (Ochi et al., Can. J. Chem. Eng., 1993, 71, 982-985)
3. CLICK OK
OK
Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

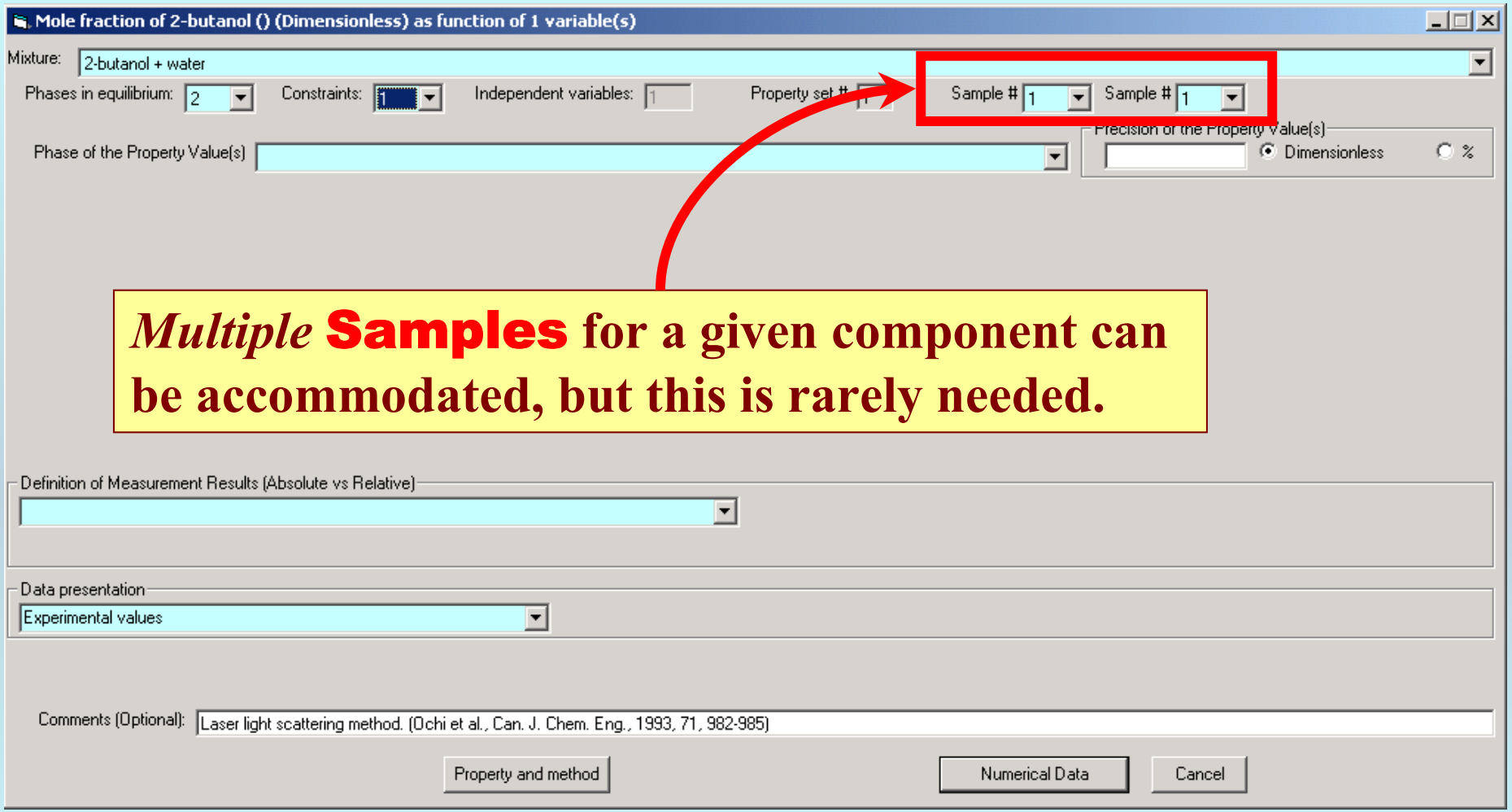


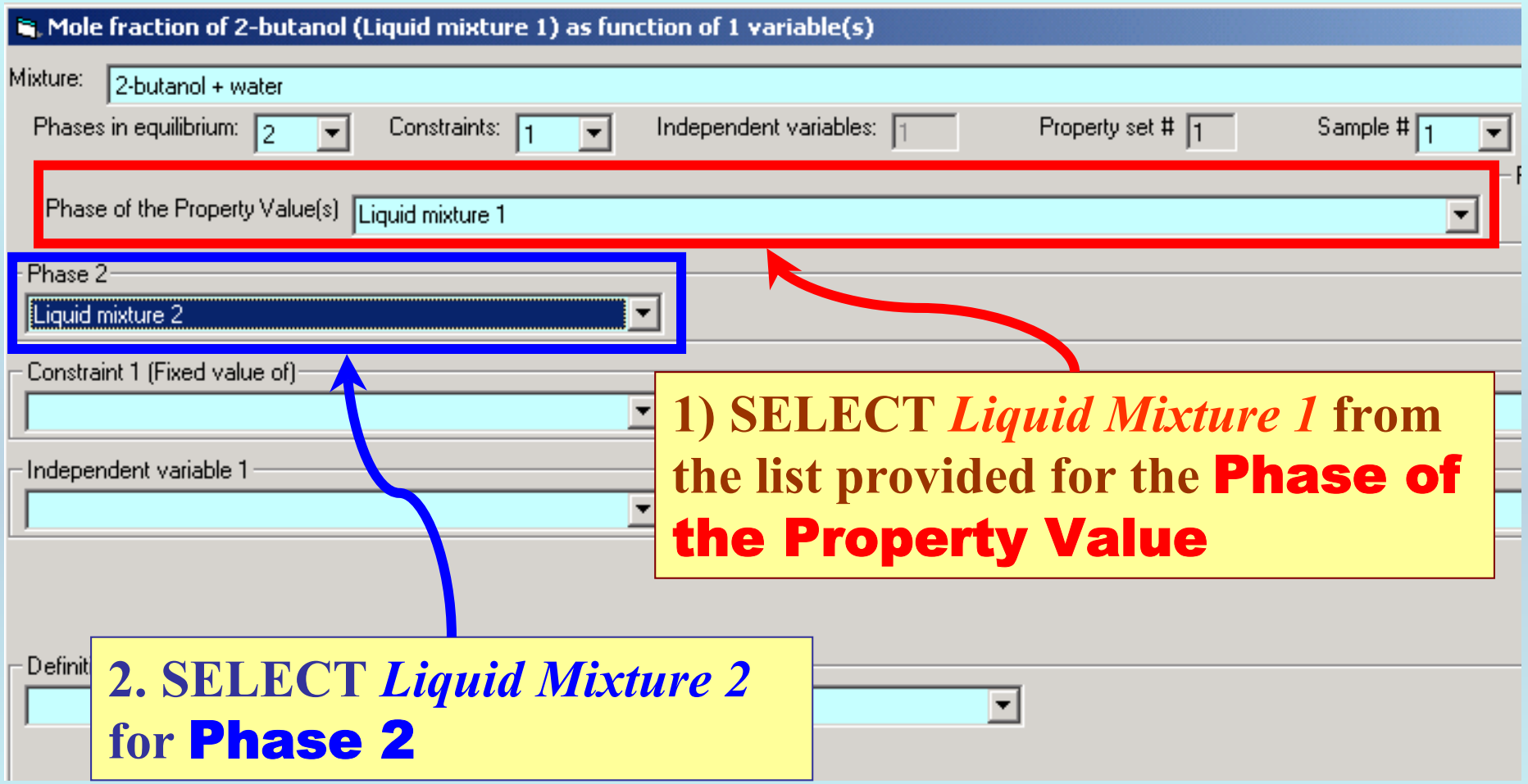
Enter the # of **Phases in equilibrium**.

There are **2** phases (liquids) in equilibrium in the case of *Mutual Solubility*.

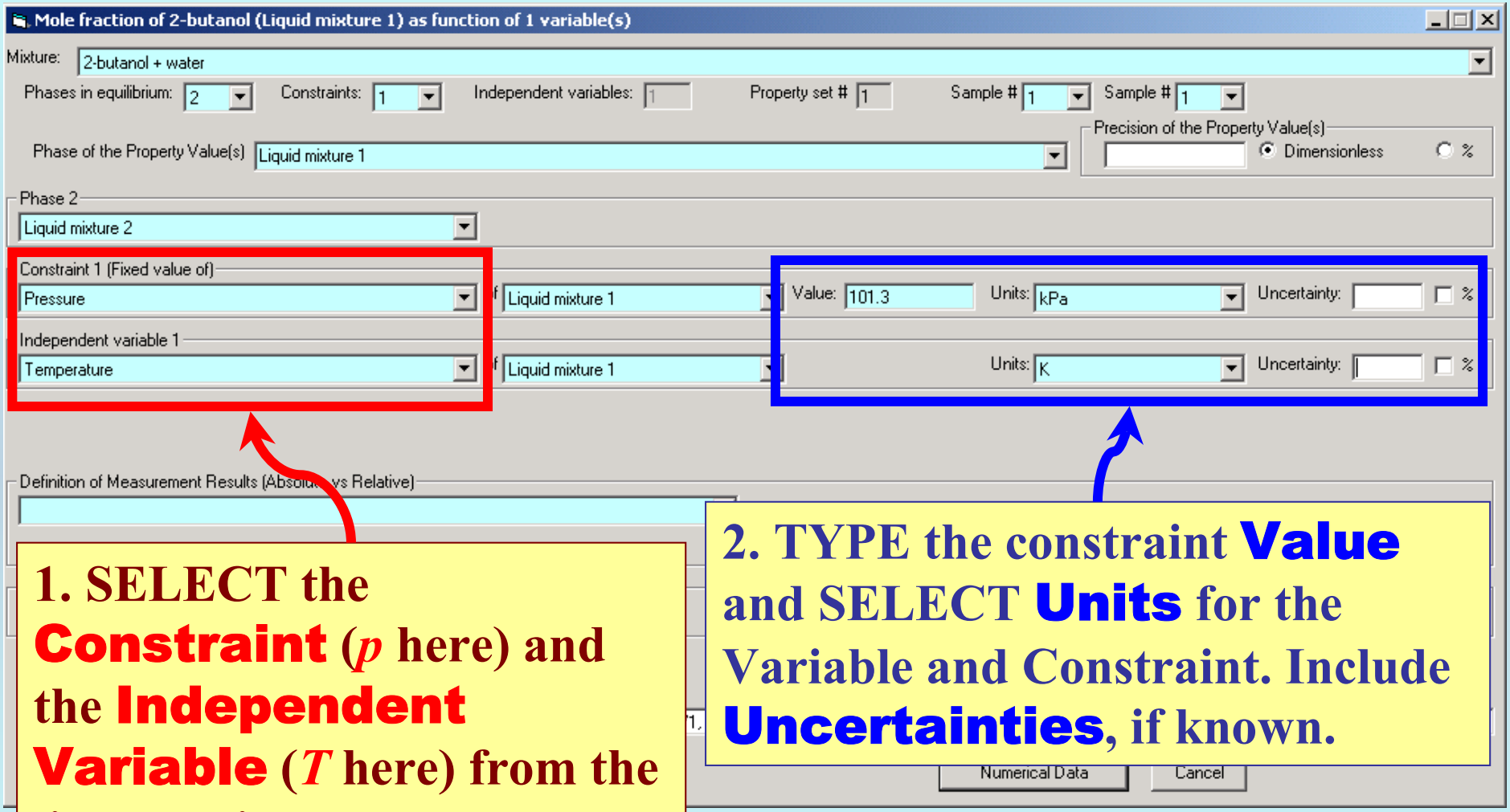
Enter the # of **Constraints**.

There is **1** constraint in the present example; *pressure = 101 kPa*.


Mole fraction of 2-butanol () (Dimensionless) as function of 1 variable(s)
Mixture:
2-butanol + water
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
Dimensionless
%
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):
Laser light scattering method. (Ochi et al., Can. J. Chem. Eng., 1993, 71, 982-985)
Property and method
Numerical Data
Cancel


Mole fraction of 2-butanol (Liquid mixture 1) as function of 1 variable(s)
Mixture:
2-butanol + water
Phases in equilibrium:
2
Constraints:
1
Independent variables:
1
Property set #
1
Sample #
1
Phase of the Property Value(s)
Liquid mixture 1
Phase 2
Liquid mixture 2
Constraint 1 (Fixed value of)
Independent variable 1
Definit
1) SELECT Liquid Mixture 1 from the list provided for the Phase of the Property Value
2. SELECT Liquid Mixture 2 for Phase 2

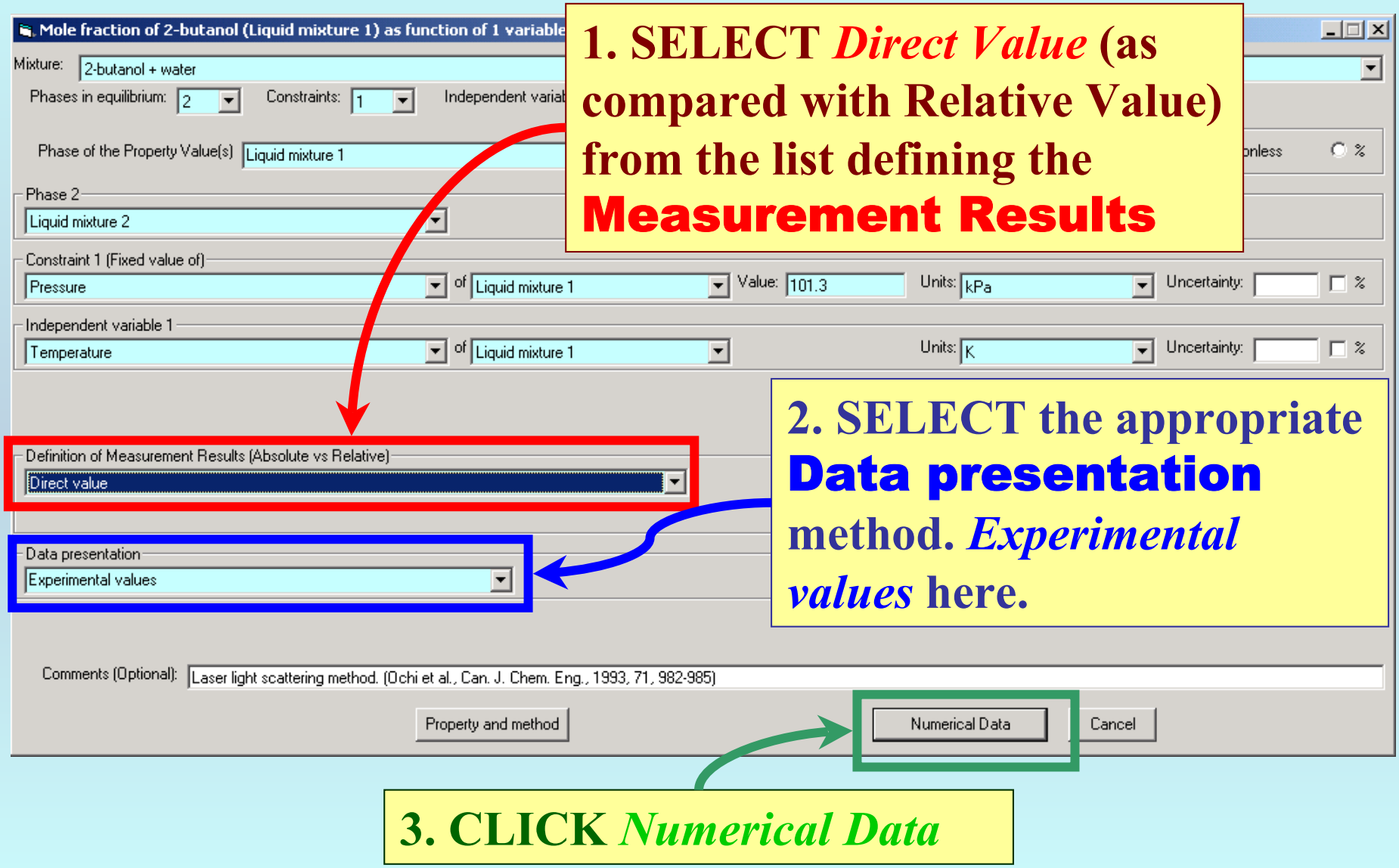
Specification of constraints, constraint values, and constraint units



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

2. TYPE the constraint **Value** and SELECT **Units** for the Variable and Constraint. Include **Uncertainties**, if known.

Measurement definition and Data presentation



Mole fraction of 2-butanol (Dimensionless) as function of 1 variable(s)

File Edit Action Help

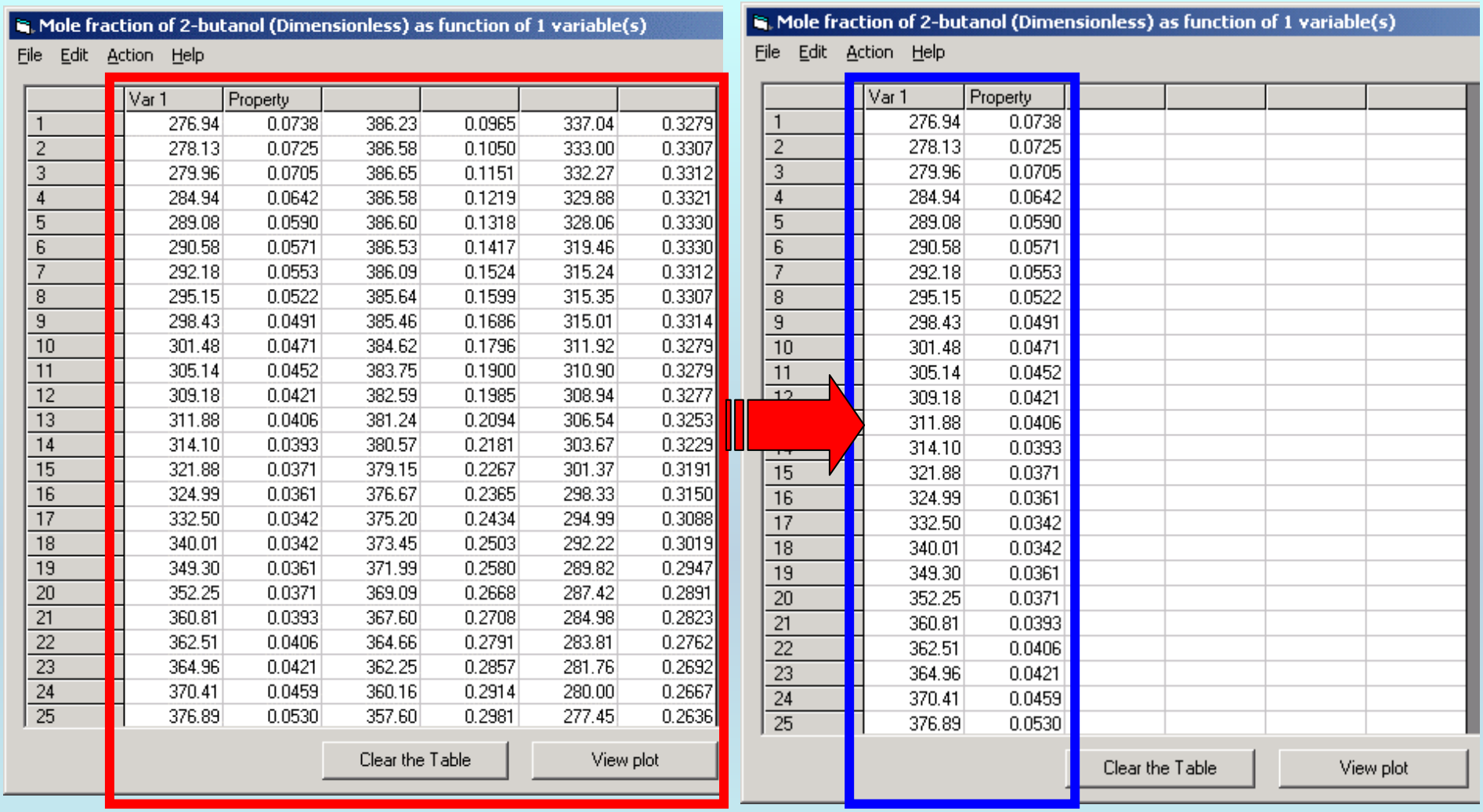
	Var 1	Property				
1	276.94	0.0738	386.23	0.0965	337.04	0.3279
2	278.13	0.0725	386.58	0.1050	333.00	0.3307
3	279.96	0.0705	386.65	0.1151	332.27	0.3312
4	284.94	0.0642	386.58	0.1219	329.88	0.3321
5	289.08	0.0590	386.60	0.1318	328.06	0.3330
6	290.58	0.0571	386.53	0.1417	319.46	0.3330
7	292.18	0.0553	386.09	0.1524	315.24	0.3312
8	295.15	0.0522	385.64	0.1599	315.35	0.3307
9	298.43	0.0491	385.46	0.1686	315.01	0.3314
10	301.48	0.0471	384.62	0.1796	311.92	0.3279
11	305.14	0.0452	383.75	0.1900	310.90	0.3279
12	309.18	0.0421	382.59	0.1985	308.94	0.3277
13	311.88	0.0406	381.24	0.2094	306.54	0.3253
14	314.10	0.0393	380.57	0.2181	303.67	0.3229
15	321.88	0.0371	379.15	0.2267	301.37	0.3191
16	324.99	0.0361	376.67	0.2365	298.33	0.3150
17	332.50	0.0342	375.20	0.2434	294.99	0.3088
18	340.01	0.0342	373.45	0.2503	292.22	0.3019
19	349.30	0.0361	371.99	0.2580	289.82	0.2947
20	352.25	0.0371	369.09	0.2668	287.42	0.2891
21	360.81	0.0393	367.60	0.2708	284.98	0.2823
22	362.51	0.0406	364.66	0.2791	283.81	0.2762
23	364.96	0.0421	362.25	0.2857	281.76	0.2692
24	370.41	0.0459	360.16	0.2914	280.00	0.2667
25	376.89	0.0530	357.60	0.2981	277.45	0.2636

Table 1. Experimental Cloud Point Results for 2-Butanol (1) + Water (2)

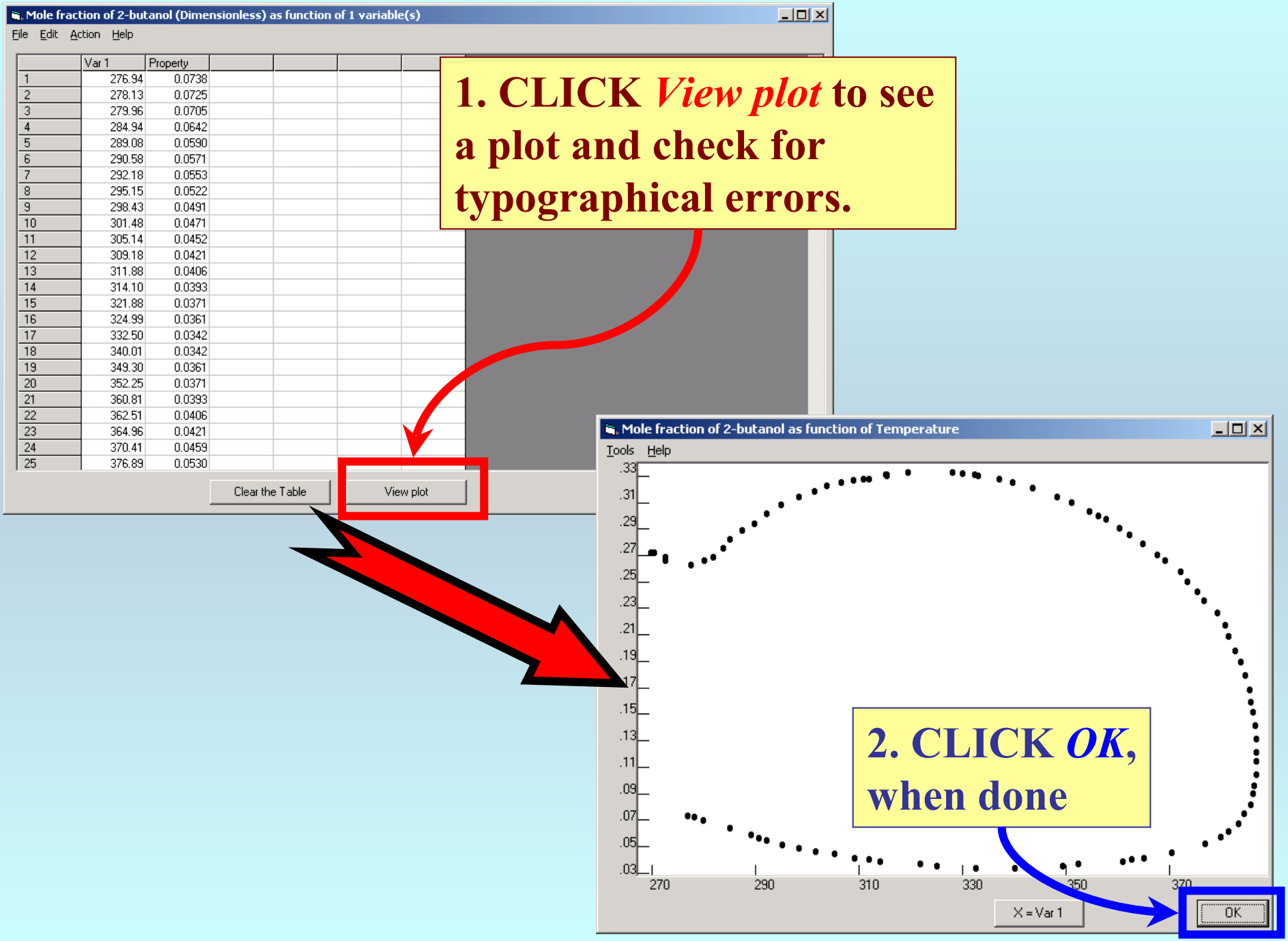
T/K	x_1[a]	T/K	x_1[a]	T/K	x_1[a]
276.94	0.0738	386.23	0.0965	337.04	0.3279
278.13	0.0725	386.58	0.1050	333.00	0.3307
279.96	0.0705	386.65[b]	0.1151[b]	332.27	0.3312
284.94	0.0642	386.58	0.1219	329.88	0.3321
289.08	0.0590	386.60	0.1318	328.06	0.3330
290.58	0.0571	386.53	0.1417	319.46	0.3330
292.18	0.0553	386.09	0.1524	315.24	0.3312
295.15	0.0522	385.64	0.1599	315.35	0.3307
298.43	0.0491	385.46	0.1686	315.01	0.3314
301.48	0.0471	384.62	0.1796	311.92	0.3279
305.14	0.0452	383.75	0.1900	310.90	0.3279
309.18	0.0421	382.59	0.1985	308.94	0.3277
311.88	0.0406	381.24	0.2094	306.54	0.3253
314.10	0.0393	380.57	0.2181	303.67	0.3229
321.88	0.0371	379.15	0.2267	301.37	0.3191
324.99	0.0361	376.67	0.2365	298.33	0.3150
332.50	0.0342	375.20	0.2434	294.99	0.3088
340.01	0.0342	373.45	0.2503	292.22	0.3019
349.30	0.0361	371.99	0.2580	289.82	0.2947
352.25	0.0371	369.09	0.2668	287.42	0.2891
360.81	0.0393	367.60	0.2708	284.98	0.2823
362.51	0.0406	364.66	0.2791	283.81	0.2762
364.96	0.0421	362.25	0.2857	281.76	0.2692
370.41	0.0459	360.16	0.2914	280.00	0.2667
376.89	0.0530	357.60	0.2981	277.45	0.2636
379.76	0.0573	356.10	0.3003	272.65	0.2667
381.25	0.0621	354.34	0.3036	272.51	0.2692
383.23	0.0680	351.02	0.3104	270.52	0.2726
384.39	0.0751	348.24	0.3150	269.75	0.2726
385.63	0.0820	343.40	0.3211		
386.04	0.0908	339.63	0.3253		

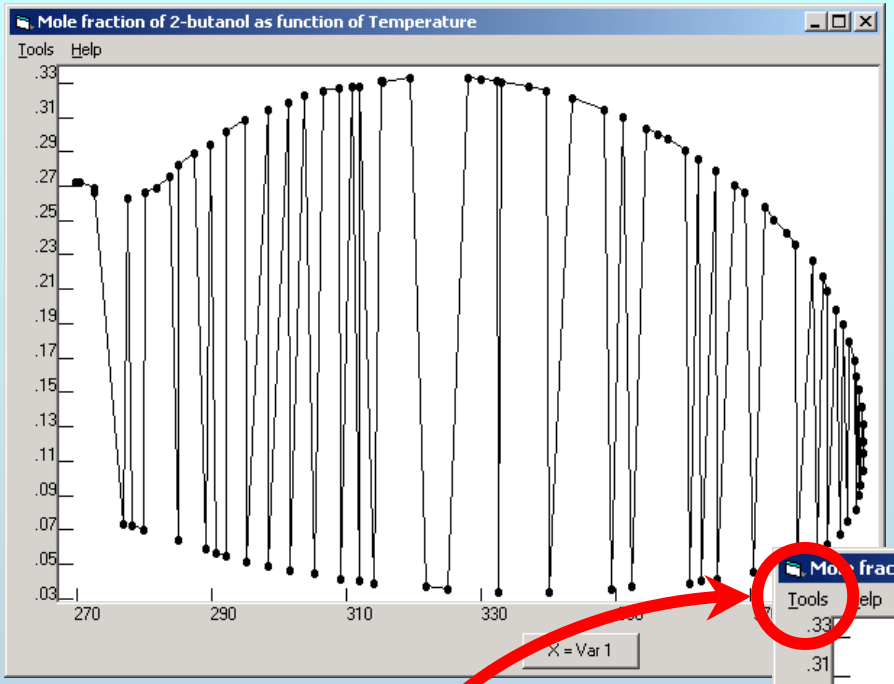
[a] Mole fraction of 2-butanol. [b] The upper critical solution point.

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

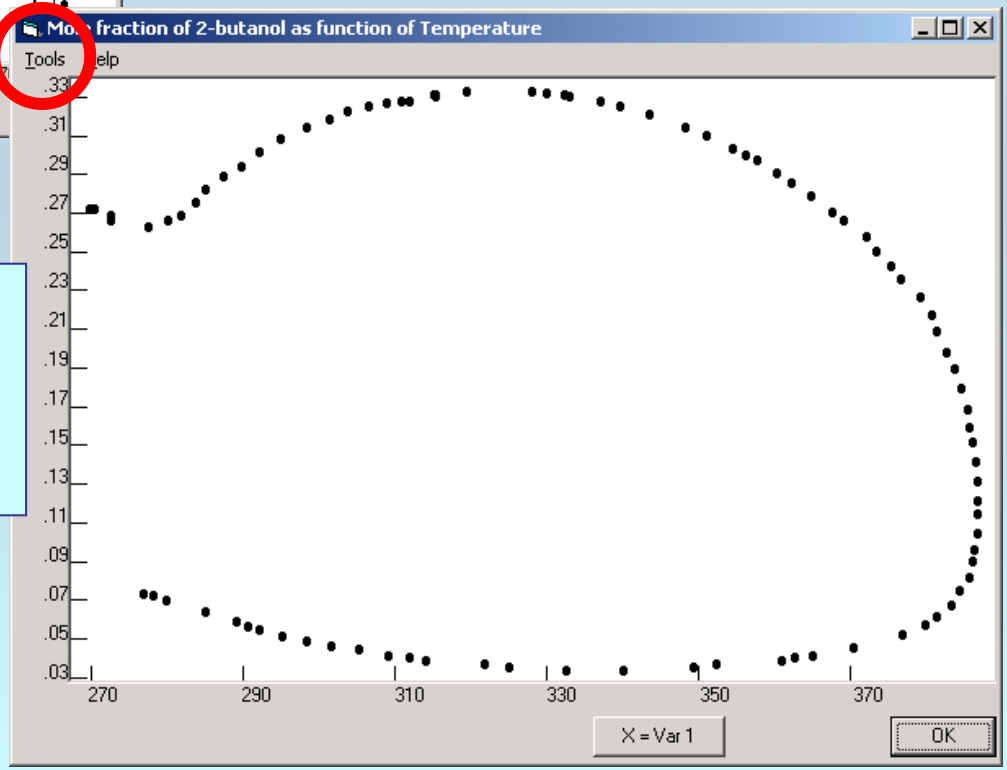


NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)

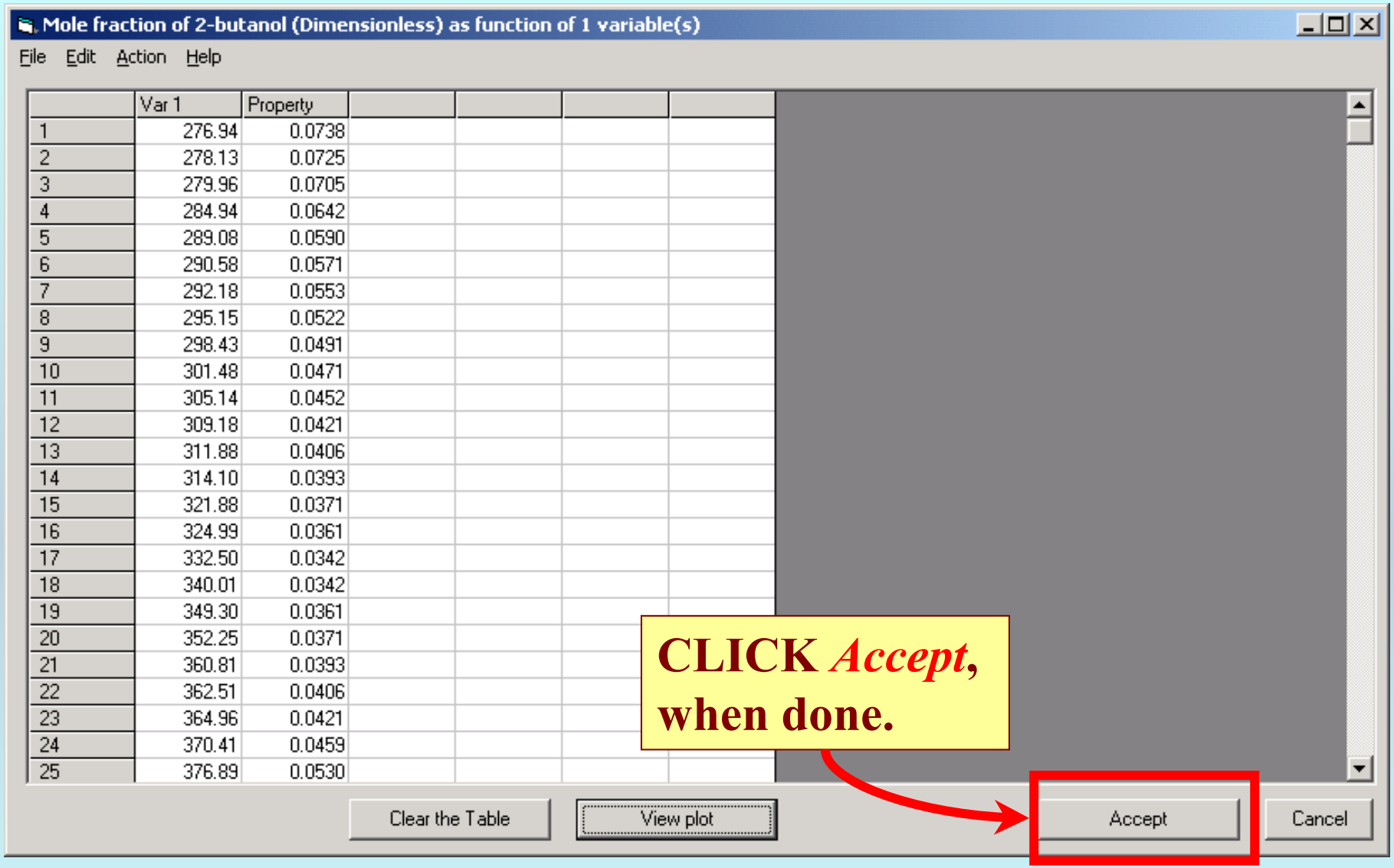

Mole fraction of 2-butanol (Dimensionless) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 276.94 0.0738
2 278.13 0.0725
3 279.96 0.0705
4 284.94 0.0642
5 289.08 0.0590
6 290.58 0.0571
7 292.18 0.0553
8 295.15 0.0522
9 298.43 0.0491
10 301.48 0.0471
11 305.14 0.0452
12 309.18 0.0421
13 311.88 0.0406
14 314.10 0.0393
15 321.88 0.0371
16 324.99 0.0361
17 332.50 0.0342
18 340.01 0.0342
19 349.30 0.0361
20 352.25 0.0371
21 360.81 0.0393
22 362.51 0.0406
23 364.96 0.0421
24 370.41 0.0459
25 376.89 0.0530
Clear the Table
View plot
1. CLICK View plot to see a plot and check for typographical errors.
Mole fraction of 2-butanol as function of Temperature
Tools Help
.33
.31
.29
.27
.25
.23
.21
.19
.17
.15
.13
.11
.09
.07
.05
.03
270
290
310
330
350
370
X = Var 1
OK
2. CLICK OK, when done

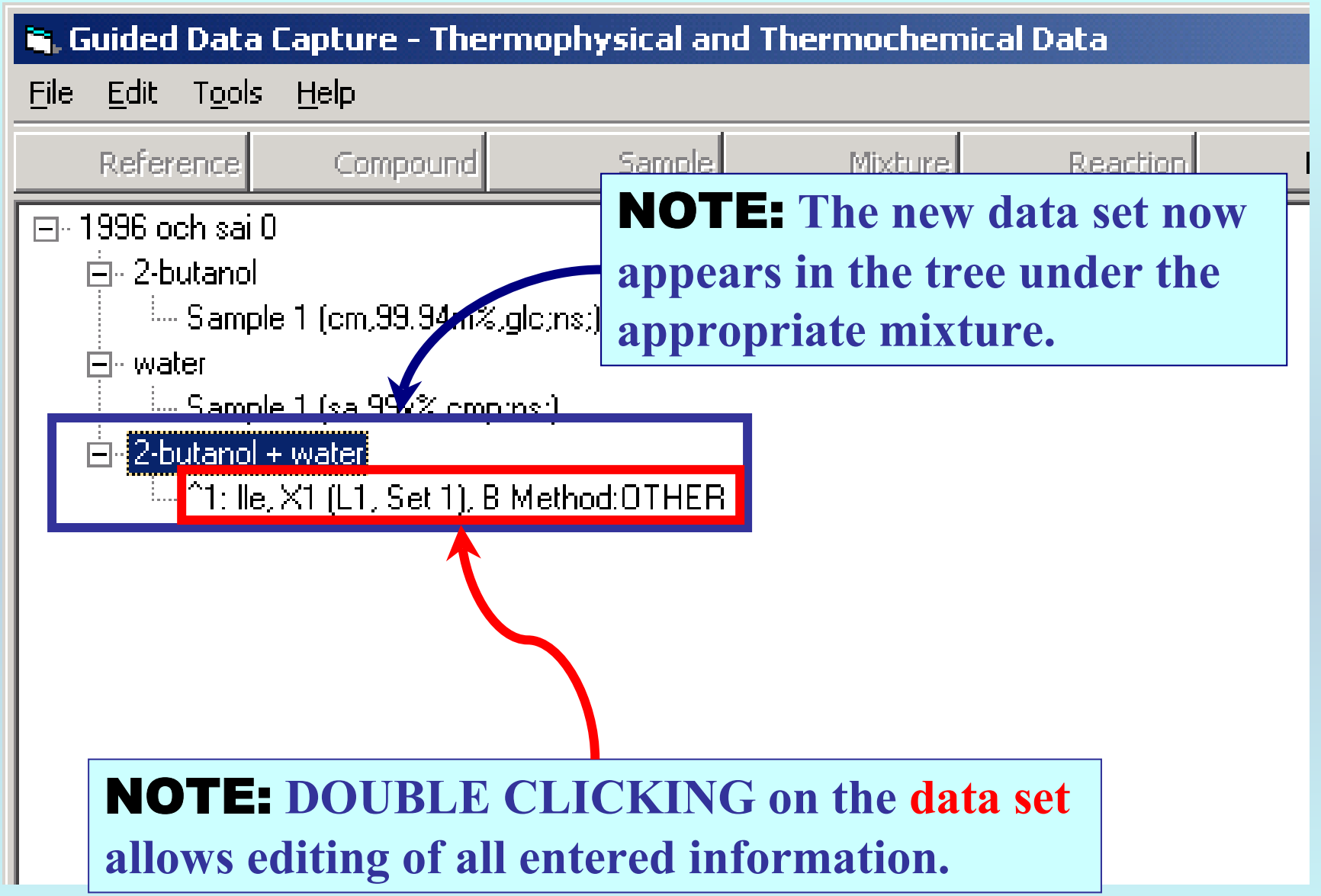


NOTE: The software automatically connects the data points with lines.



If these are not helpful (*as here*), they can be cleared in the **Tools** menu.


Mole fraction of 2-butanol (Dimensionless) as function of 1 variable(s)
File Edit Action Help
Var 1 Property
1 276.94 0.0738
2 278.13 0.0725
3 279.96 0.0705
4 284.94 0.0642
5 289.08 0.0590
6 290.58 0.0571
7 292.18 0.0553
8 295.15 0.0522
9 298.43 0.0491
10 301.48 0.0471
11 305.14 0.0452
12 309.18 0.0421
13 311.88 0.0406
14 314.10 0.0393
15 321.88 0.0371
16 324.99 0.0361
17 332.50 0.0342
18 340.01 0.0342
19 349.30 0.0361
20 352.25 0.0371
21 360.81 0.0393
22 362.51 0.0406
23 364.96 0.0421
24 370.41 0.0459
25 376.89 0.0530
Clear the Table
View plot
Accept
Cancel
CLICK Accept, when done.


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample Mixture Reaction
1996 och sai 0
2-butanol
Sample 1 (cm,99.94m%,glc;ns;)
water
2-butanol + water
^1: Ile, X1 (L1, Set 1), B Method:OTHER
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.**