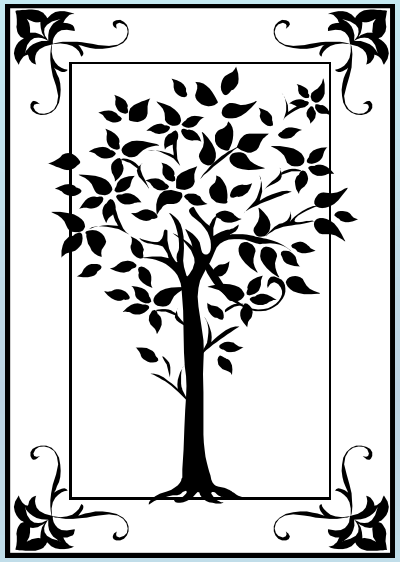
METADATA AND NUMERICAL DATA CAPTURE:
Liquid-Liquid Equilibria
(3-Component: Tie-Line Data)

Guided Data Capture (GDC)



This tutorial decribes
METADATA AND NUMERICAL DATA CAPTURE:
for **Liquid-Liquid Equilibria (3 components)**
TIE-LINE DATA
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*, 1007−1011

Liquid−Liquid Equilibria of Octane + (Benzene or Toluene or *m*-Xylene) + Sulfolane at 323.15, 348.15, and 373.15 K

Wen-Churng Lin* and Nien-Hsin Kao

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Equilibrium tie line data have been determined at 323.15 K, 348.15 K, and 373.15 K for the ternary liquid−liquid equilibria (LLE) of octane + (benzene or toluene or *m*-xylene) + sulfolane systems. The relative mutual solubility of benzene is higher than that of toluene or *m*-xylene in octane + sulfolane mixtures. The tie line data were correlated with the NRTL and UNIQUAC models. The calculated values based on the NRTL model were found to be better than those based on the UNIQUAC model; the average root-mean-square deviation between the phase composition obtained from experiment and that from calculation was 0.49 for NRTL compared to 0.53 for UNIQUAC. The values of selectivity and the distribution coefficient were derived from the equilibrium data at different temperatures.

LLE data for (octane + benzene + sulfolane) at p = 101.3 kPa

Table 1. Experimental LLE Data, Selectivities, S, and Distribution Coefficients, κ, for the System

	octane-rich phase			sulfolane-rich phase				
T/K	x_{11}	x_{21}	x_{31}	x_{13}	x_{23}	x_{33}	S	κ
	Octane (1) + Benzene (2) + Sulfolane (3)							
323.15	0.997	0.000	0.003	0.006	0.000	0.994		
	0.905	0.091	0.004	0.013	0.045	0.942	34	0.49
	0.815	0.178	0.007	0.017	0.106	0.877	29	0.60
	0.732	0.259	0.009	0.017	0.162	0.821	27	0.63
	0.657	0.336	0.007	0.016	0.216	0.768	26	0.64
	0.550	0.434	0.016	0.016	0.289	0.695	23	0.67
	0.335	0.625	0.040	0.028	0.477	0.495	9	0.76
	0.279	0.668	0.053	0.034	0.535	0.431	7	0.80
348.15	0.993	0.000	0.007	0.011	0.000	0.989		
	0.897	0.093	0.010	0.013	0.044	0.943	33	0.47
	0.813	0.175	0.012	0.014	0.100	0.886	35	0.57
	0.712	0.272	0.016	0.019	0.176	0.805	24	0.65
	0.604	0.376	0.020	0.027	0.248	0.725	15	0.66
	0.475	0.491	0.034	0.033	0.349	0.618	10	0.71
	0.408	0.548	0.044	0.041	0.409	0.550	7	0.75
	0.328	0.617	0.055	0.046	0.490	0.464	6	0.79
373.15	0.992	0.000	0.008	0.013	0.000	0.987		
	0.893	0.093	0.014	0.013	0.044	0.943	32	0.48
	0.812	0.173	0.015	0.015	0.097	0.888	30	0.56
	0.720	0.259	0.021	0.015	0.140	0.845	26	0.54
	0.646	0.334	0.020	0.028	0.214	0.758	15	0.64
	0.476	0.477	0.047	0.032	0.281	0.687	9	0.59
	0.399	0.532	0.069	0.050	0.398	0.552	6	0.74
	0.300	0.598	0.102	0.057	0.482	0.461	4	0.81

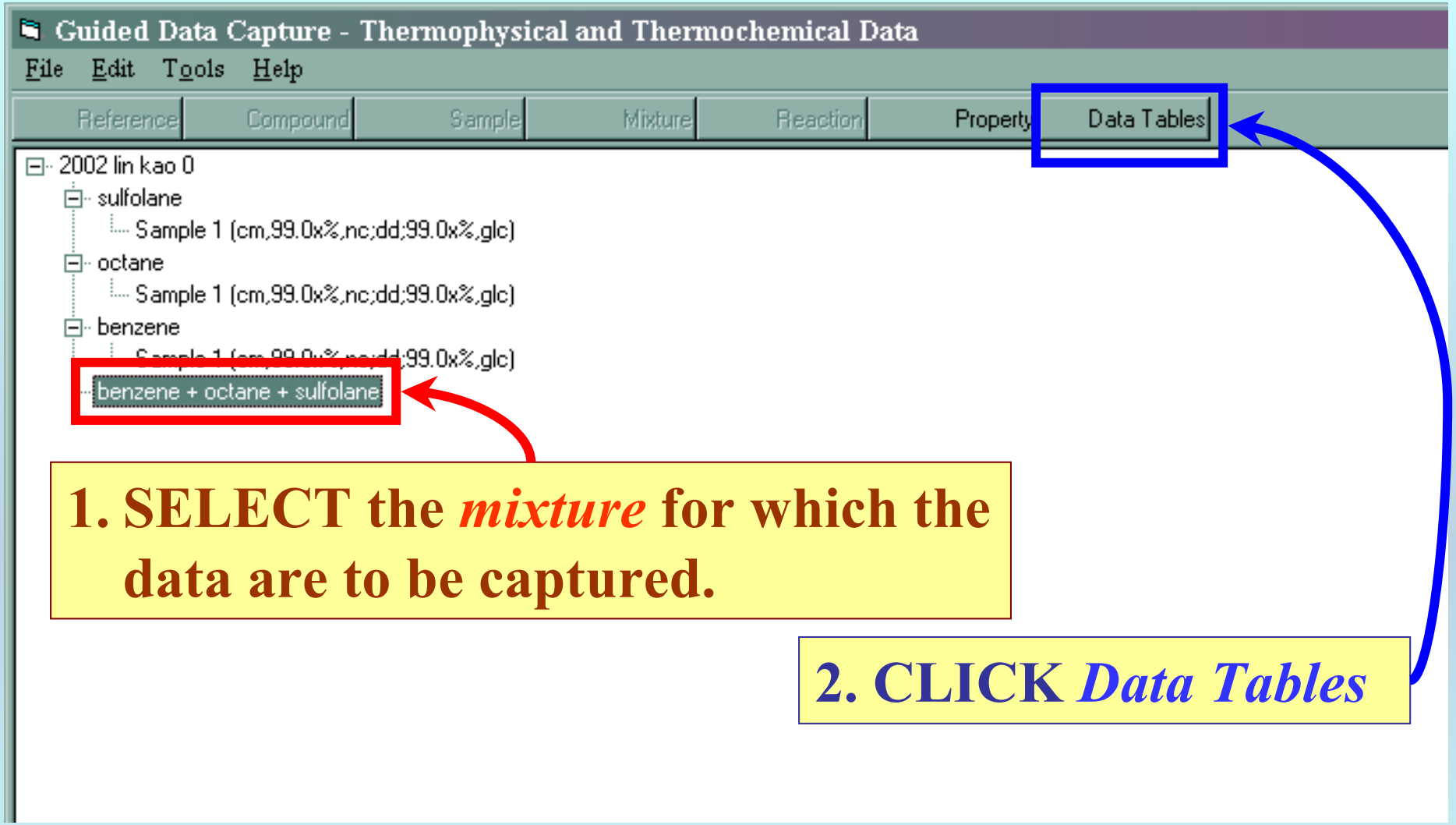
This data set is considered here.

Experimental Method Info:

The sample analysis was performed using a Hewlett-Packard Model 5890 gas chromatograph equipped with a flame ionization detector and a HP Ultra 1 column (cross-linked methyl silicone gum, 25 m × 3.2 × 10^{-4} m × 5.2 × 10^{-7} m film thickness)

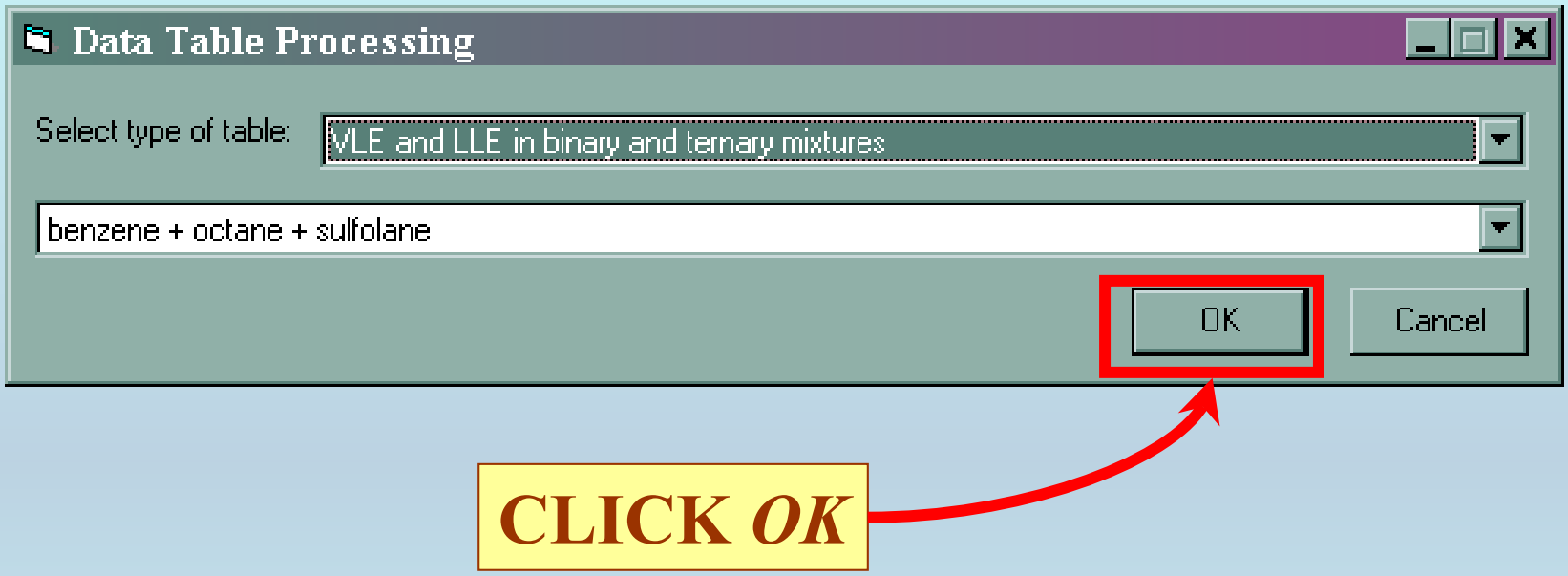
Mass fraction measurements were reproducible to within ±0.005.

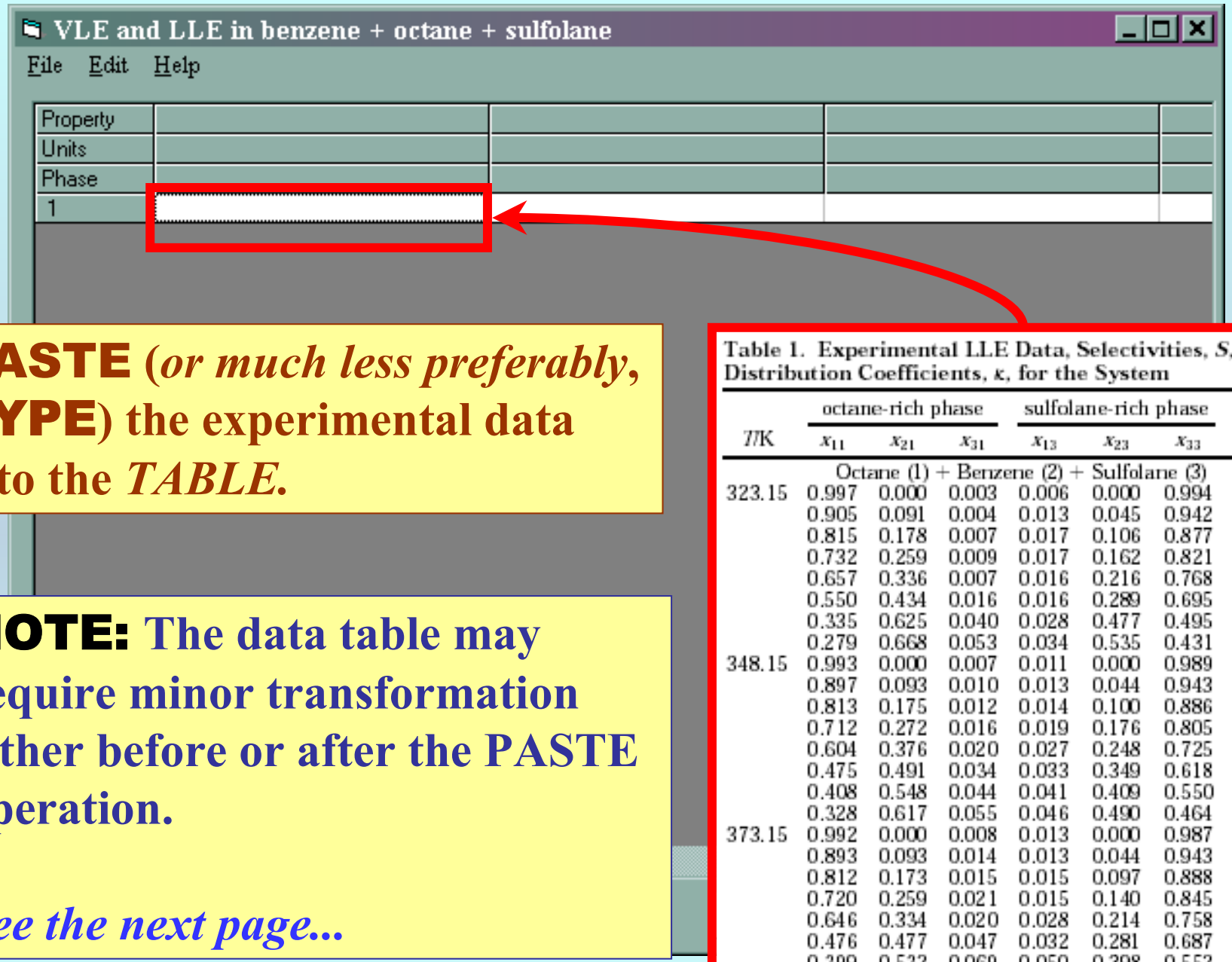
Temperatures were controlled to ±0.03 K.



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

This form appears:





PASTE (*or much less preferably*, **TYPE**) **the experimental data into the *TABLE*.**

NOTE: **The data table may require minor transformation either before or after the PASTE operation.**

See the next page...

Table 1. Experimental LLE Data, Selectivities, S, and Distribution Coefficients, κ, for the System

	octane-rich phase			sulfolane-rich phase				
T/K	x_{11}	x_{21}	x_{31}	x_{13}	x_{23}	x_{33}	S	κ
	Octane (1) + Benzene (2) + Sulfolane (3)							
323.15	0.997	0.000	0.003	0.006	0.000	0.994		
	0.905	0.091	0.004	0.013	0.045	0.942	34	0.49
	0.815	0.178	0.007	0.017	0.106	0.877	29	0.60
	0.732	0.259	0.009	0.017	0.162	0.821	27	0.63
	0.657	0.336	0.007	0.016	0.216	0.768	26	0.64
	0.550	0.434	0.016	0.016	0.289	0.695	23	0.67
	0.335	0.625	0.040	0.028	0.477	0.495	9	0.76
	0.279	0.668	0.053	0.034	0.535	0.431	7	0.80
348.15	0.993	0.000	0.007	0.011	0.000	0.989		
	0.897	0.093	0.010	0.013	0.044	0.943	33	0.47
	0.813	0.175	0.012	0.014	0.100	0.886	33	0.57
	0.712	0.272	0.016	0.019	0.176	0.805	24	0.65
	0.604	0.376	0.020	0.027	0.248	0.725	15	0.66
	0.475	0.491	0.034	0.033	0.349	0.618	10	0.71
	0.408	0.548	0.044	0.041	0.409	0.550	7	0.75
	0.328	0.617	0.055	0.046	0.490	0.464	6	0.79
373.15	0.992	0.000	0.008	0.013	0.000	0.987		
	0.893	0.093	0.014	0.013	0.044	0.943	32	0.48
	0.812	0.173	0.015	0.015	0.097	0.888	30	0.56
	0.720	0.259	0.021	0.015	0.140	0.845	26	0.54
	0.646	0.334	0.020	0.028	0.214	0.758	15	0.64
	0.476	0.477	0.047	0.032	0.281	0.687	9	0.59
	0.399	0.532	0.069	0.050	0.398	0.552	6	0.75
	0.300	0.598	0.102	0.057	0.482	0.461	4	0.81

Table Transformation

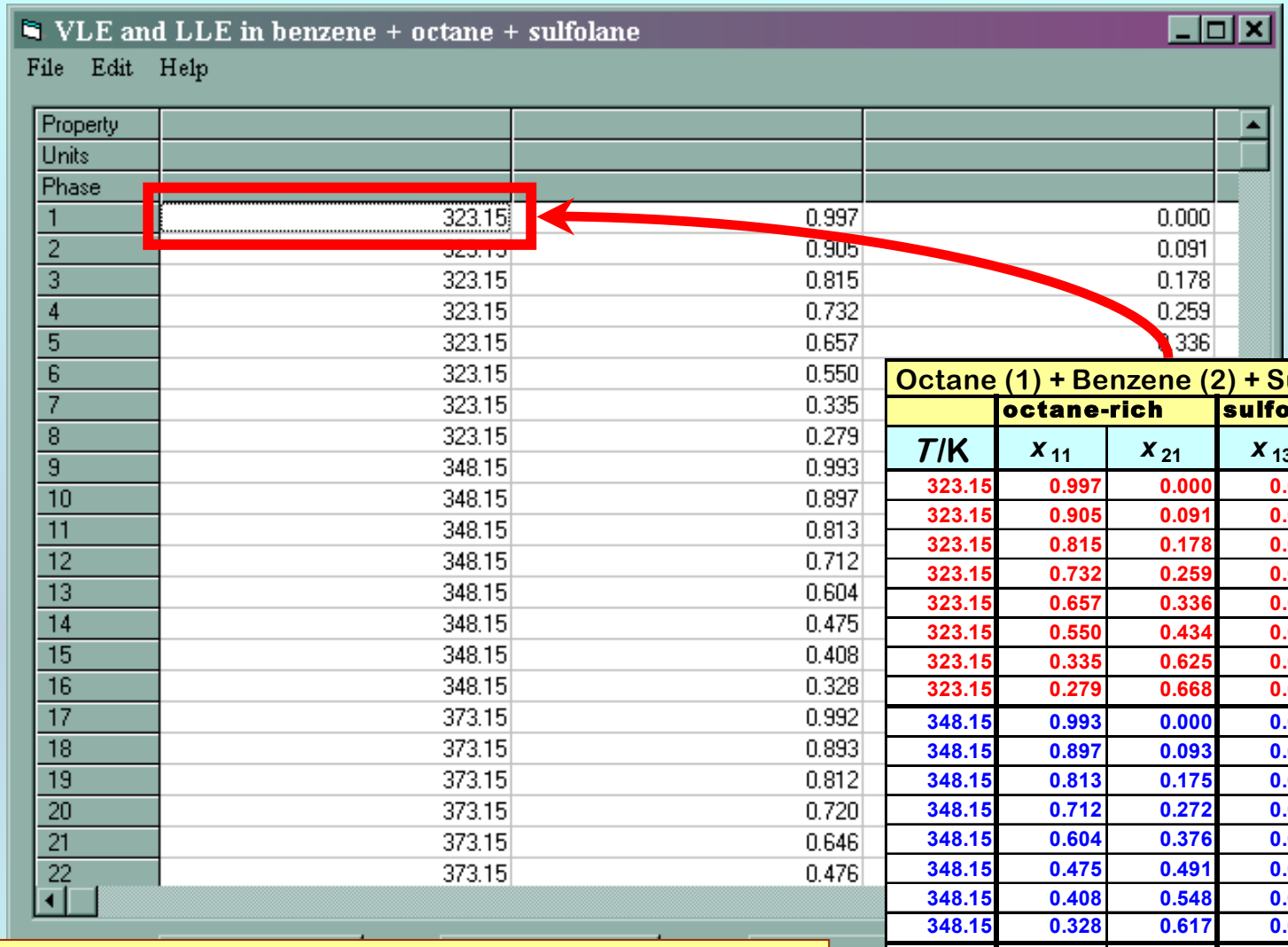
Table 1. Experimental LLE Data, Selectivities, S, and Distribution Coefficients, κ, for the System

	octane-rich phase			sulfolane-rich phase				
T/K	x_{11}	x_{21}	x_{31}	x_{13}	x_{23}	x_{33}	S	κ
	Octane (1) + Benzene (2) + Sulfolane (3)							
323.15	0.997	0.000	0.003	0.006	0.000	0.994		
	0.905	0.091	0.004	0.013	0.045	0.942	34	0.49
	0.815	0.178	0.007	0.017	0.106	0.877	29	0.60
	0.732	0.259	0.009	0.017	0.162	0.821	27	0.63
	0.657	0.336	0.007	0.016	0.216	0.768	26	0.64
	0.550	0.434	0.016	0.016	0.289	0.695	23	0.67
	0.335	0.625	0.040	0.028	0.477	0.495	9	0.76
	0.279	0.668	0.053	0.034	0.535	0.431	7	0.80
348.15	0.993	0.000	0.007	0.011	0.000	0.989		
	0.897	0.093	0.010	0.013	0.044	0.943	33	0.47
	0.813	0.175	0.012	0.014	0.100	0.886	33	0.57
	0.712	0.272	0.016	0.019	0.176	0.805	24	0.65
	0.604	0.376	0.020	0.027	0.248	0.725	15	0.66
	0.475	0.491	0.034	0.033	0.349	0.618	10	0.71
	0.408	0.548	0.044	0.041	0.409	0.550	7	0.75
	0.328	0.617	0.055	0.046	0.490	0.464	6	0.79
373.15	0.992	0.000	0.008	0.013	0.000	0.987		
	0.893	0.093	0.014	0.013	0.044	0.943	32	0.48
	0.812	0.173	0.015	0.015	0.097	0.888	30	0.56
	0.720	0.259	0.021	0.015	0.140	0.845	26	0.54
	0.646	0.334	0.020	0.028	0.214	0.758	15	0.64
	0.476	0.477	0.047	0.032	0.281	0.687	9	0.59
	0.399	0.532	0.069	0.050	0.398	0.552	6	0.73
	0.300	0.598	0.102	0.057	0.482	0.461	4	0.81

Octane (1) + Benzene (2) + Sulfolane (3)

	octane-rich		sulfolane-rich	
T/K	x_{11}	x_{21}	x_{13}	x_{23}
323.15	0.997	0.000	0.006	0.000
323.15	0.905	0.091	0.013	0.045
323.15	0.815	0.178	0.017	0.106
323.15	0.732	0.259	0.017	0.162
323.15	0.657	0.336	0.016	0.216
323.15	0.550	0.434	0.016	0.289
323.15	0.335	0.625	0.028	0.477
323.15	0.279	0.668	0.034	0.535
348.15	0.993	0.000	0.011	0.000
348.15	0.897	0.093	0.013	0.044
348.15	0.813	0.175	0.014	0.100
348.15	0.712	0.272	0.019	0.176
348.15	0.604	0.376	0.027	0.248
348.15	0.475	0.491	0.033	0.349
348.15	0.408	0.548	0.041	0.409
348.15	0.328	0.617	0.046	0.490
373.15	0.992	0.000	0.013	0.000
373.15	0.893	0.093	0.013	0.044
373.15	0.812	0.173	0.015	0.097
373.15	0.720	0.259	0.015	0.140
373.15	0.646	0.334	0.028	0.214
373.15	0.476	0.477	0.032	0.281
373.15	0.399	0.532	0.050	0.398
373.15	0.300	0.598	0.057	0.482

Note: The GDC software includes many useful table operations. See the *HELP* menu on the screen for details. Alternatively, any spreadsheet software (e.g., EXCEL) can be used.

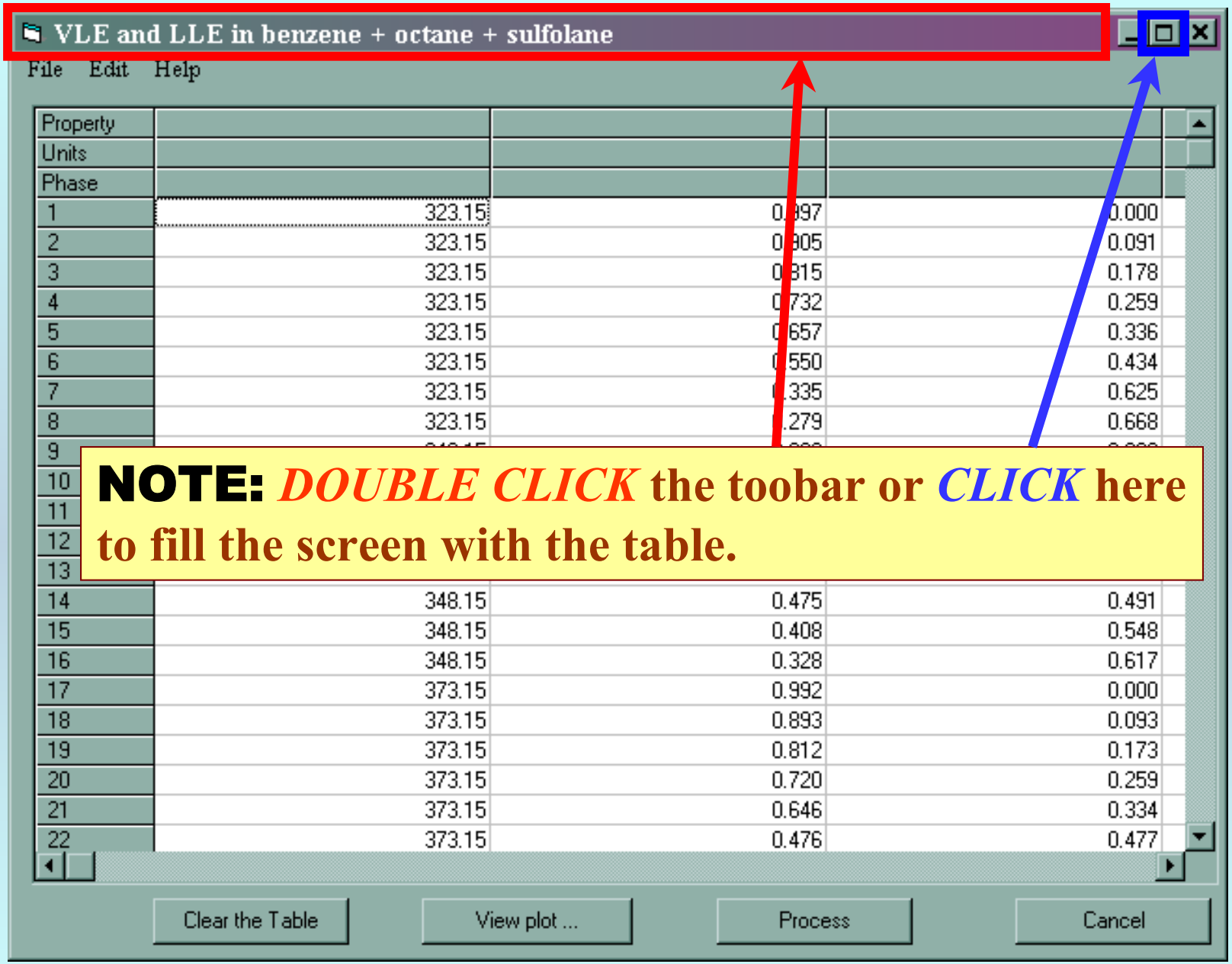


Octane (1) + Benzene (2) + Sulfolane (3)

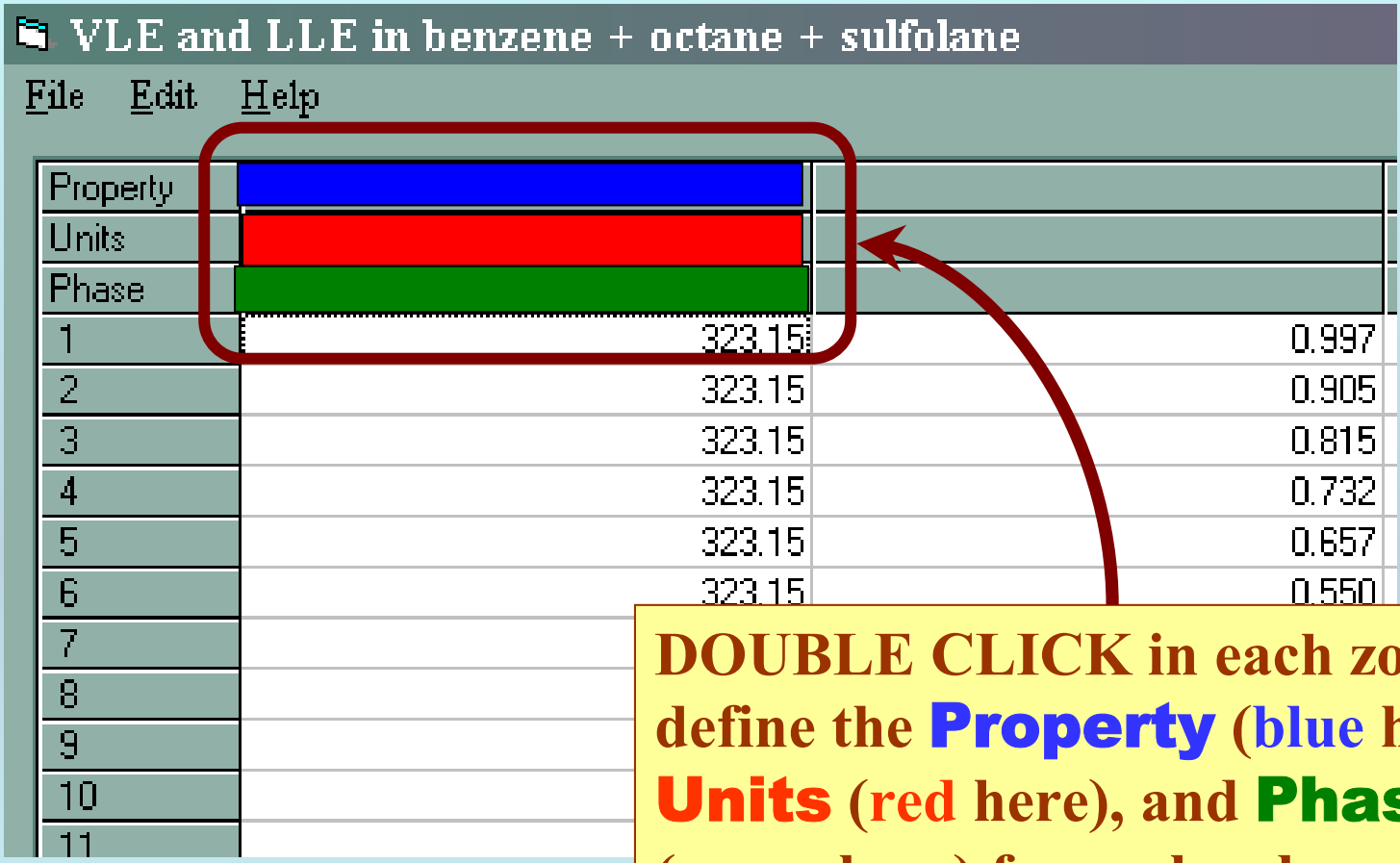
	octane-rich		sulfolane-rich	
T/K	x_{11}	x_{21}	x_{13}	x_{23}
323.15	0.997	0.000	0.006	0.000
323.15	0.905	0.091	0.013	0.045
323.15	0.815	0.178	0.017	0.106
323.15	0.732	0.259	0.017	0.162
323.15	0.657	0.336	0.016	0.216
323.15	0.550	0.434	0.016	0.289
323.15	0.335	0.625	0.028	0.477
323.15	0.279	0.668	0.034	0.535
348.15	0.993	0.000	0.011	0.000
348.15	0.897	0.093	0.013	0.044
348.15	0.813	0.175	0.014	0.100
348.15	0.712	0.272	0.019	0.176
348.15	0.604	0.376	0.027	0.248
348.15	0.475	0.491	0.033	0.349
348.15	0.408	0.548	0.041	0.409
348.15	0.328	0.617	0.046	0.490
373.15	0.992	0.000	0.013	0.000
373.15	0.893	0.093	0.013	0.044
373.15	0.812	0.173	0.015	0.097
373.15	0.720	0.259	0.015	0.140
373.15	0.646	0.334	0.028	0.214
373.15	0.476	0.477	0.032	0.281
373.15	0.399	0.532	0.050	0.398
373.15	0.300	0.598	0.057	0.482

NOTE: This is the result of the *PASTE* operation.

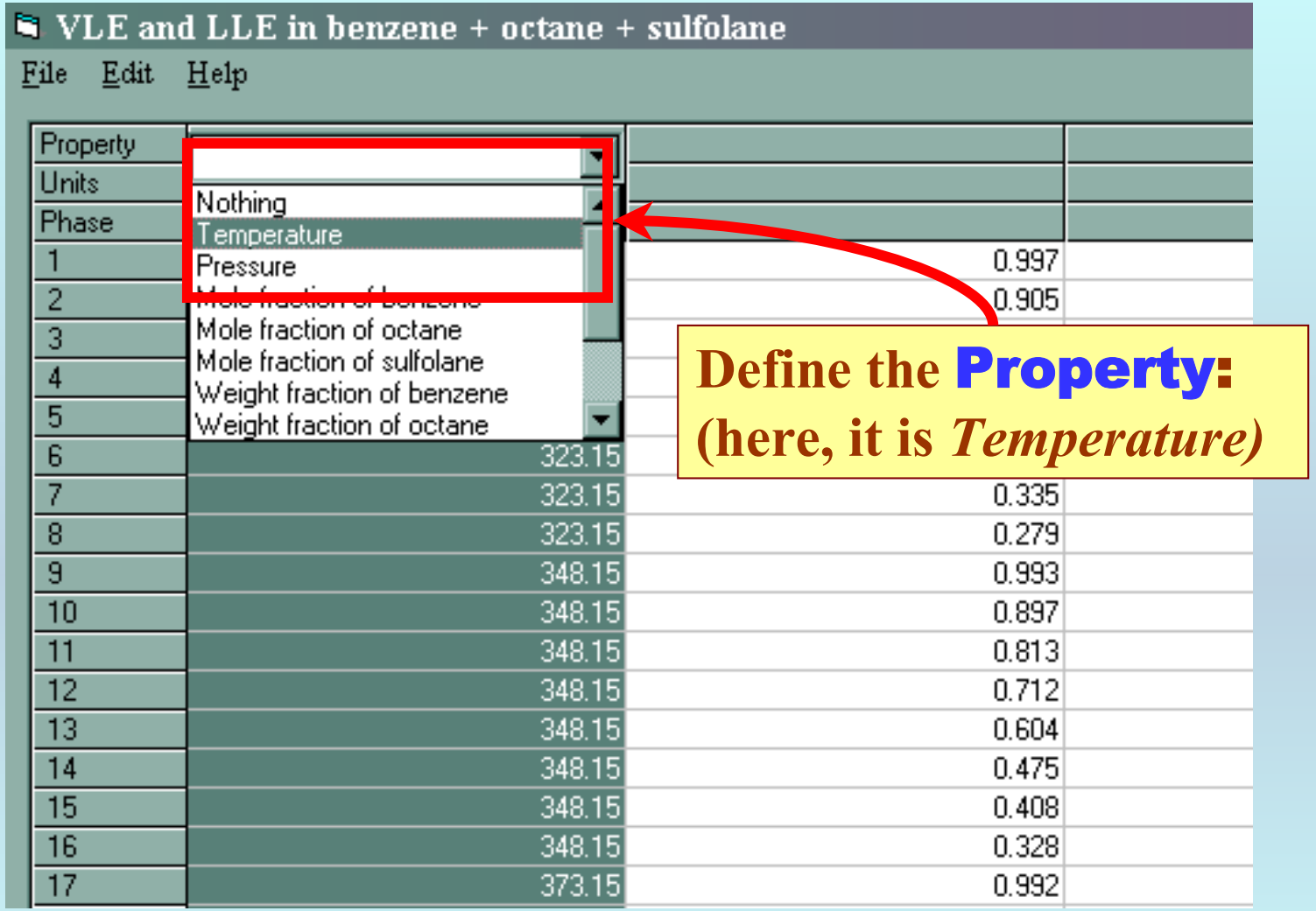
Continue with the tutorial...

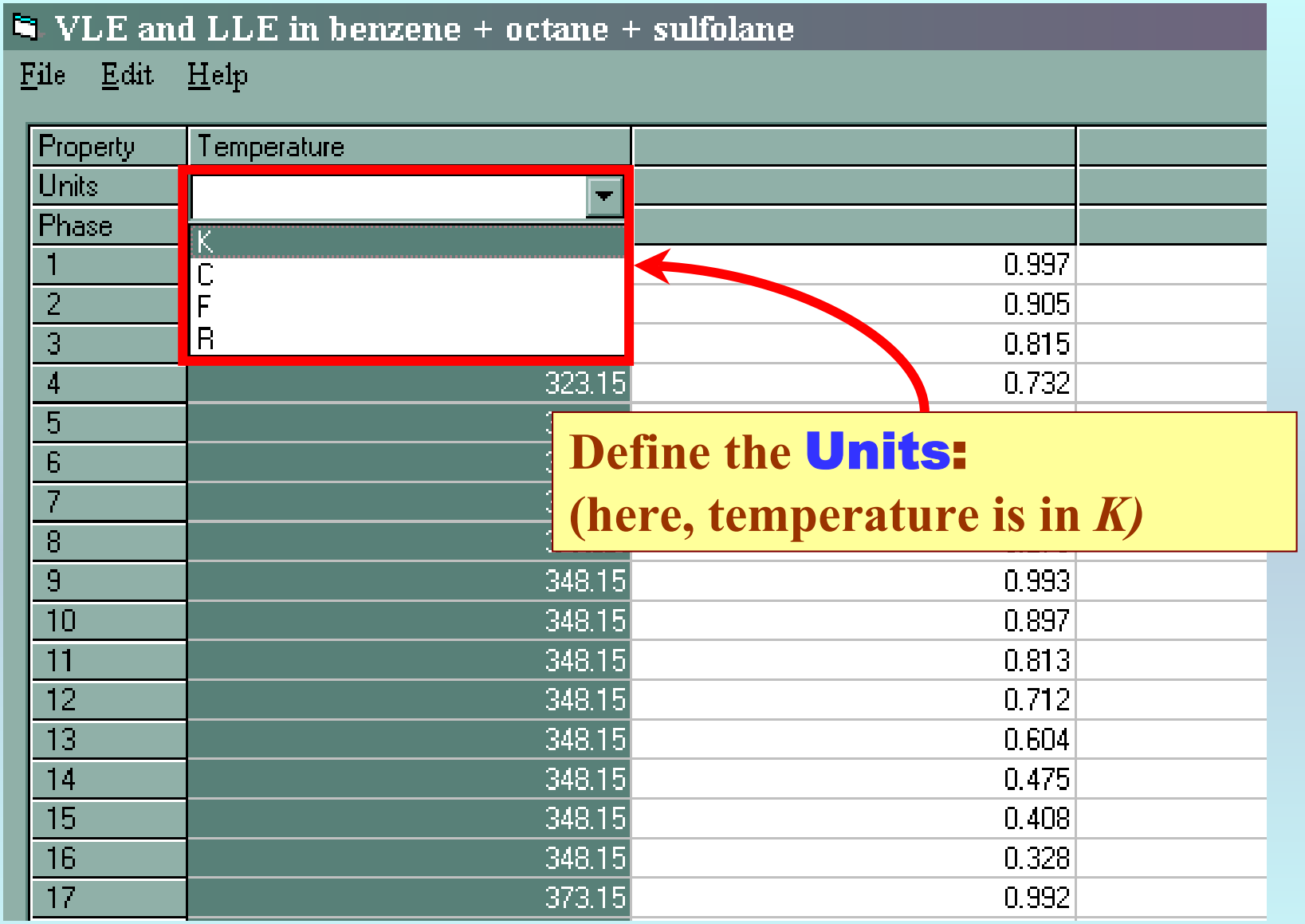

VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property
Units
Phase
1 323.15 0.897 0.000
2 323.15 0.805 0.091
3 323.15 0.715 0.178
4 323.15 0.732 0.259
5 323.15 0.657 0.336
6 323.15 0.550 0.434
7 323.15 0.335 0.625
8 323.15 0.279 0.668
14 348.15 0.475 0.491
15 348.15 0.408 0.548
16 348.15 0.328 0.617
17 373.15 0.992 0.000
18 373.15 0.893 0.093
19 373.15 0.812 0.173
20 373.15 0.720 0.259
21 373.15 0.646 0.334
22 373.15 0.476 0.477
NOTE: DOUBLE CLICK the toobar or CLICK here to fill the screen with the table.
Clear the Table
View plot ...
Process
Cancel

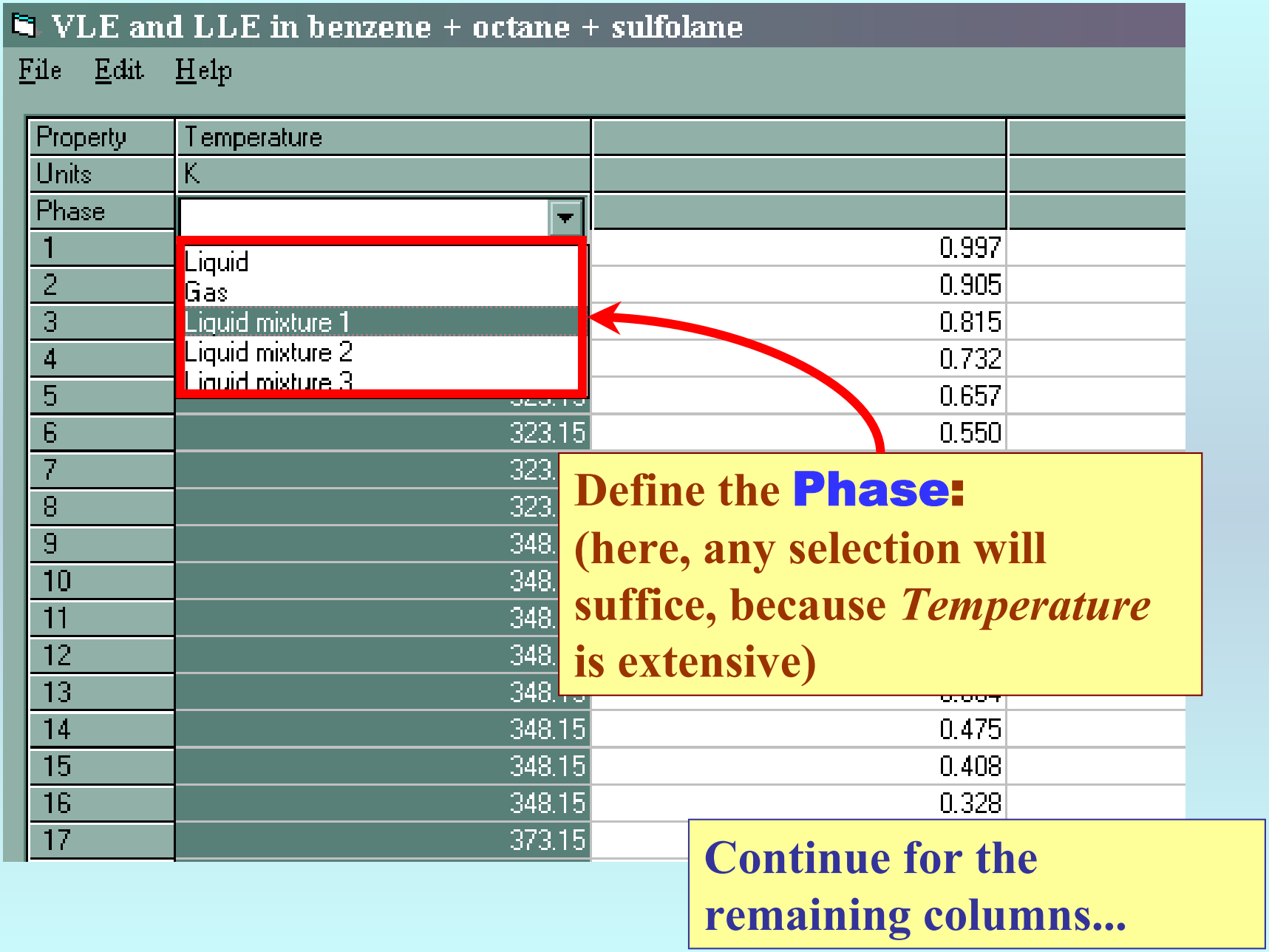
Property, Units, and Phase Definitions:

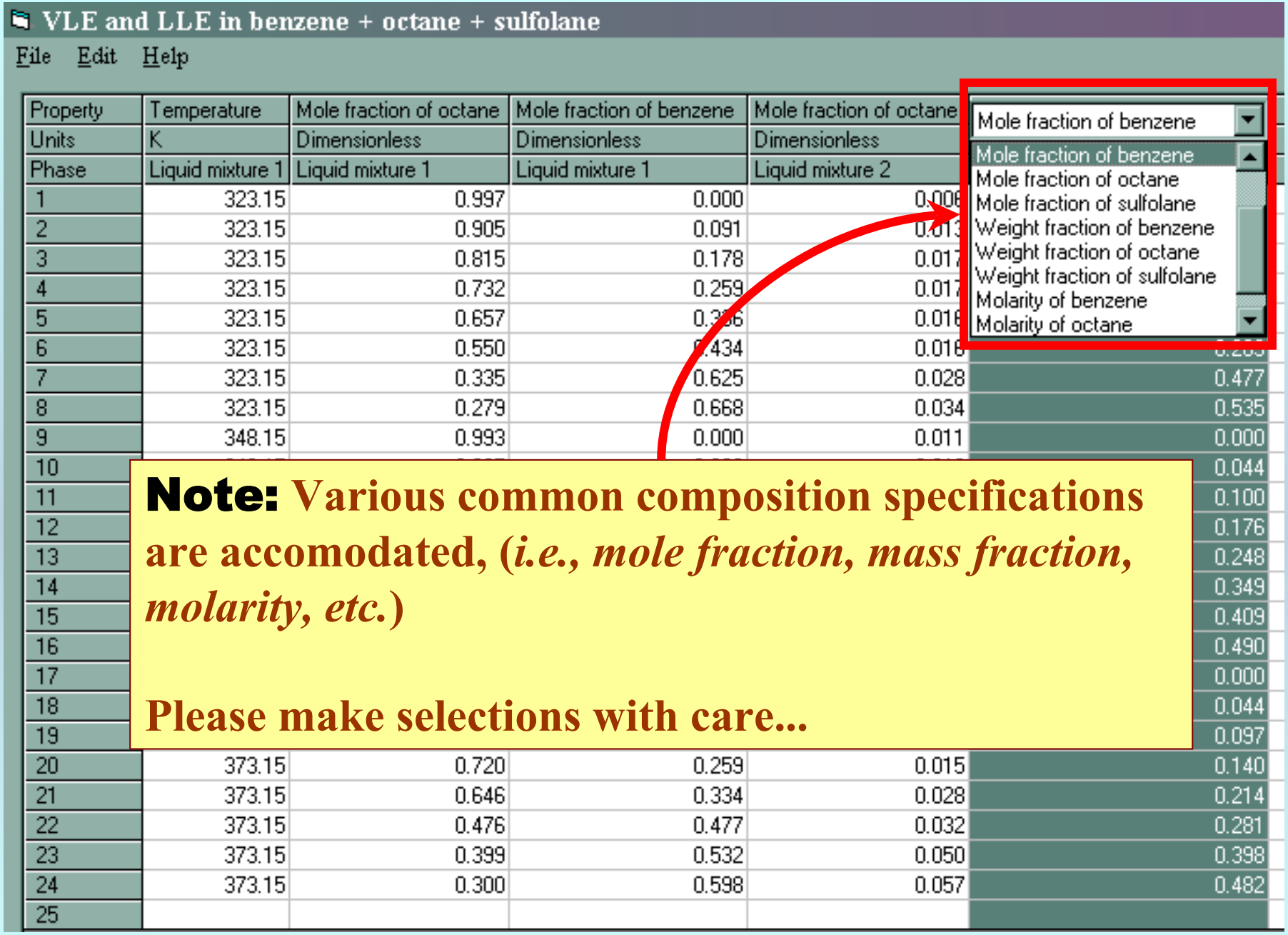


DOUBLE CLICK in each zone to define the Property (blue here), Units (red here), and Phase (green here) for each column from menus. *(See next page...)*


VLE and LLE in benzene + octane + sulfolane
File
Edit
Help
Property
Units
Phase
Nothing
Temperature
Pressure
Mole fraction of octane
Mole fraction of sulfolane
Weight fraction of benzene
Weight fraction of octane
1 0.997
2 0.905
3
4
5
6 323.15
7 323.15 0.335
8 323.15 0.279
9 348.15 0.993
10 348.15 0.897
11 348.15 0.813
12 348.15 0.712
13 348.15 0.604
14 348.15 0.475
15 348.15 0.408
16 348.15 0.328
17 373.15 0.992
Define the Property:
(here, it is Temperature)


VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property
Temperature
Units
Phase
K
C
F
R
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
323.15
348.15
348.15
348.15
348.15
348.15
348.15
348.15
348.15
373.15
0.997
0.905
0.815
0.732
0.993
0.897
0.813
0.712
0.604
0.475
0.408
0.328
0.992
Define the Units:
(here, temperature is in K)


VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property
Temperature
Units
K
Phase
Liquid
Gas
Liquid mixture 1
Liquid mixture 2
Liquid mixture 3
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
323.15
348.15
348.15
348.15
373.15
0.997
0.905
0.815
0.732
0.657
0.550
0.475
0.408
0.328
Define the Phase:
(here, any selection will suffice, because Temperature is extensive)
Continue for the remaining columns...

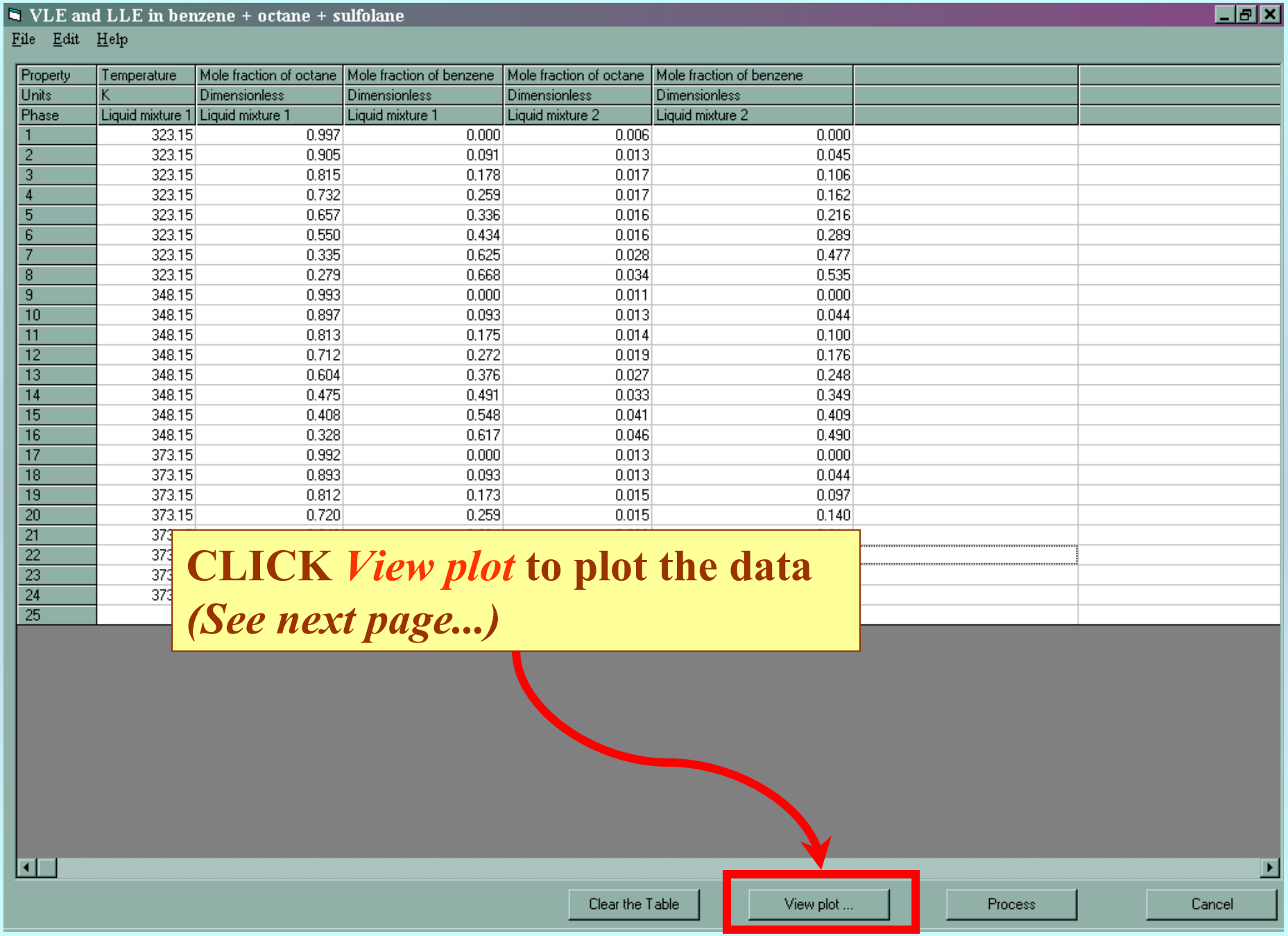

VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property | Temperature | Mole fraction of octane | Mole fraction of benzene | Mole fraction of octane
Units | K | Dimensionless | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2
1 323.15 0.997 0.000
2 323.15 0.905 0.091
3 323.15 0.815 0.178
4 323.15 0.732 0.259
5 323.15 0.657
6 323.15 0.550
7 323.15 0.335 0.625 0.028 0.477
8 323.15 0.279 0.668 0.034 0.535
9 348.15 0.993 0.000 0.011 0.000
10 0.044
11 0.100
12 0.176
13 0.248
14 0.349
15 0.409
16 0.490
17 0.000
18 0.044
19 0.097
20 373.15 0.720 0.259 0.015 0.140
21 373.15 0.646 0.334 0.028 0.214
22 373.15 0.476 0.477 0.032 0.281
23 373.15 0.399 0.532 0.050 0.398
24 373.15 0.300 0.598 0.057 0.482
25
Mole fraction of benzene
Mole fraction of benzene
Mole fraction of octane
Mole fraction of sulfolane
Weight fraction of benzene
Weight fraction of octane
Weight fraction of sulfolane
Molarity of benzene
Molarity of octane
Note: Various common composition specifications are accomodated, (i.e., mole fraction, mass fraction, molarity, etc.)
Please make selections with care...

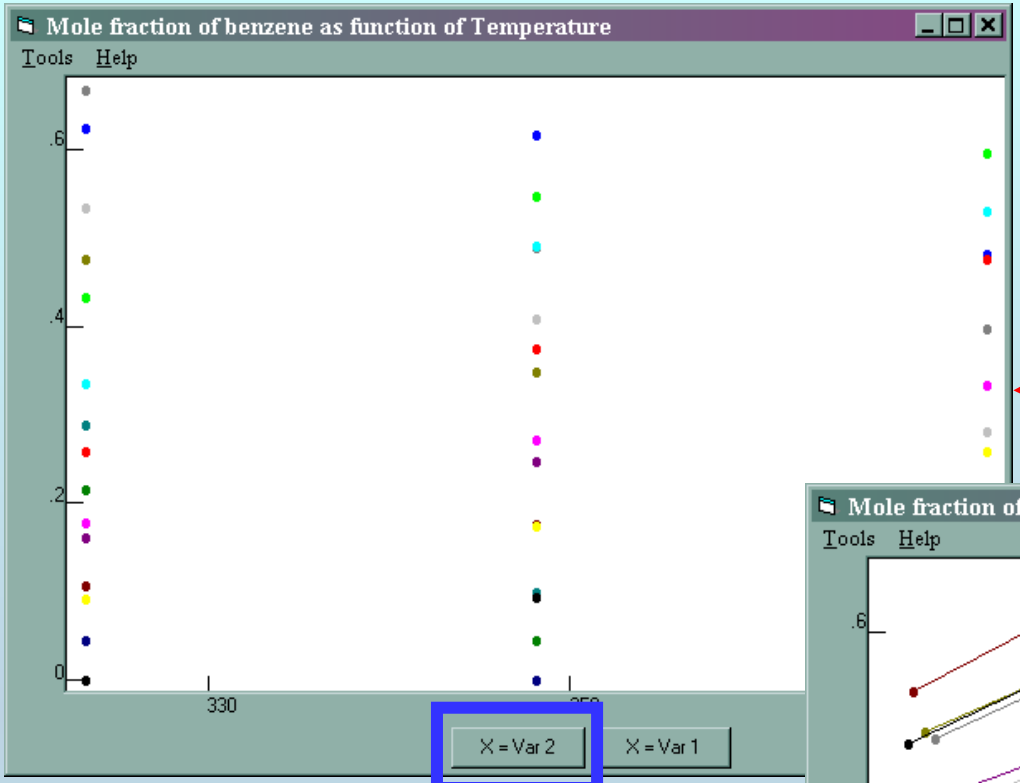
VLE and LLE in benzene + octane + sulfolane

File Edit Help

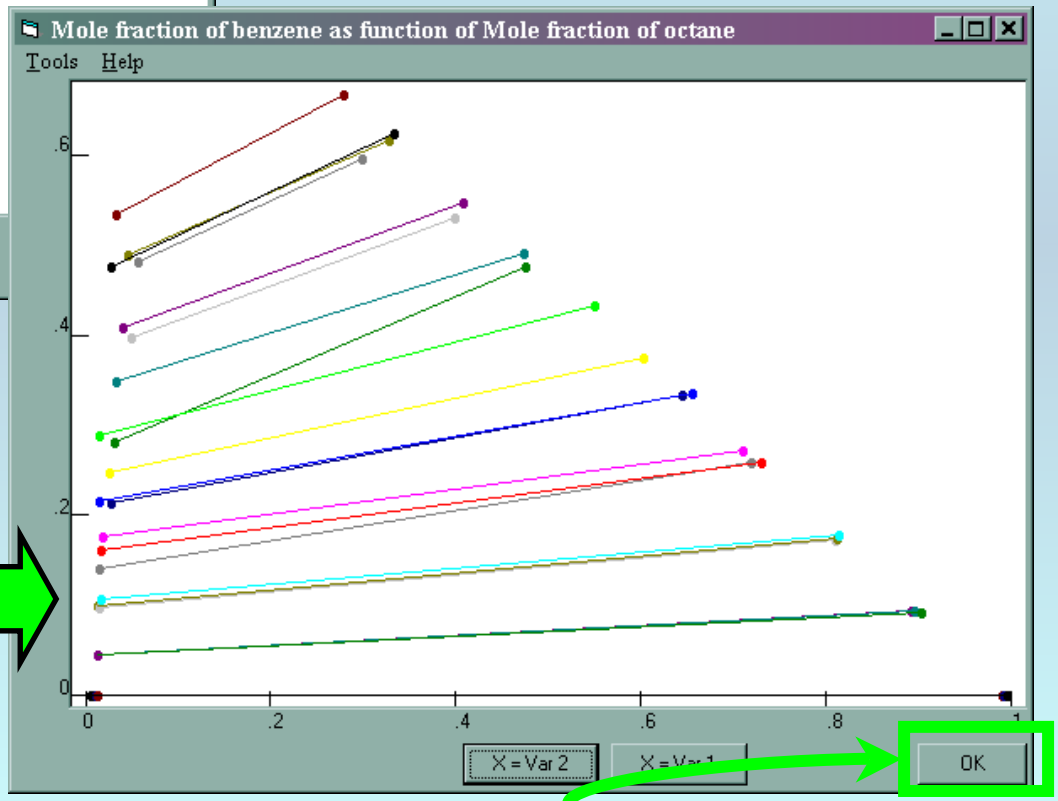
Property	Temperature	Mole fraction of octane	Mole fraction of benzene	Mole fraction of octane	Mole fraction of benzene
Units	K	Dimensionless	Dimensionless	Dimensionless	Dimensionless
Phase	Liquid mixture 1	Liquid mixture 1	Liquid mixture 1	Liquid mixture 2	Liquid mixture 2
1	323.15	0.997	0.000	0.006	0.000
2	323.15	0.905	0.091	0.013	0.045
3	323.15	0.815	0.178	0.01	0.106
4	323.15	0.7 2	0.259	0.017	0.162
5	323.15	0.657	0.33	0.016	0.216
6	323.15	0.550	0.434	0.016	0.289
7	323.15	0.335	0.63	0.028	0.477
8	323.15	0.279	0.668	0.034	0.535
9	348.15	0.993	0.000	0.011	0.000
10					0.044
11					0.100
12					0.176
13					0.248
14	348.15	0.475	0.491	0.033	0.349
15	348.15	0.408	0.548	0.041	0.409
16	348.15	0.328	0.617	0.046	0.490
17	373.15	0.992	0.000	0.013	0.000
18	373.15	0.893	0.093	0.013	0.044
19	373.15	0.812	0.173	0.015	0.097
20	373.15	0.720	0.259	0.015	0.140
21	373.15	0.646	0.334	0.028	0.214
22	373.15	0.476	0.477	0.032	0.281
23	373.15	0.399	0.532	0.050	0.398
24	373.15	0.300	0.598	0.057	0.482
25					

NOTE: ***LIQUID MIXTURE 1*** **and** ***LIQUID MIXTURE 2*** **identify the two liquid phases.**


VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property | Temperature | Mole fraction of octane | Mole fraction of benzene | Mole fraction of octane | Mole fraction of benzene
Units | K | Dimensionless | Dimensionless | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2 | Liquid mixture 2
1 323.15 0.997 0.000 0.006 0.000
2 323.15 0.905 0.091 0.013 0.045
3 323.15 0.815 0.178 0.017 0.106
4 323.15 0.732 0.259 0.017 0.162
5 323.15 0.657 0.336 0.016 0.216
6 323.15 0.550 0.434 0.016 0.289
7 323.15 0.335 0.625 0.028 0.477
8 323.15 0.279 0.668 0.034 0.535
9 348.15 0.993 0.000 0.011 0.000
10 348.15 0.897 0.093 0.013 0.044
11 348.15 0.813 0.175 0.014 0.100
12 348.15 0.712 0.272 0.019 0.176
13 348.15 0.604 0.376 0.027 0.248
14 348.15 0.475 0.491 0.033 0.349
15 348.15 0.408 0.548 0.041 0.409
16 348.15 0.328 0.617 0.046 0.490
17 373.15 0.992 0.000 0.013 0.000
18 373.15 0.893 0.093 0.013 0.044
19 373.15 0.812 0.173 0.015 0.097
20 373.15 0.720 0.259 0.015 0.140
21
22
23
24
25
CLICK View plot to plot the data
(See next page...)
Clear the Table
View plot ...
Process
Cancel



A plot like this may appear initially.



CLICK here to change the x-axis to provide an alternative view.

CLICK *OK*, when done viewing.

VLE and LLE in benzene + octane + sulfolane

File Edit Help

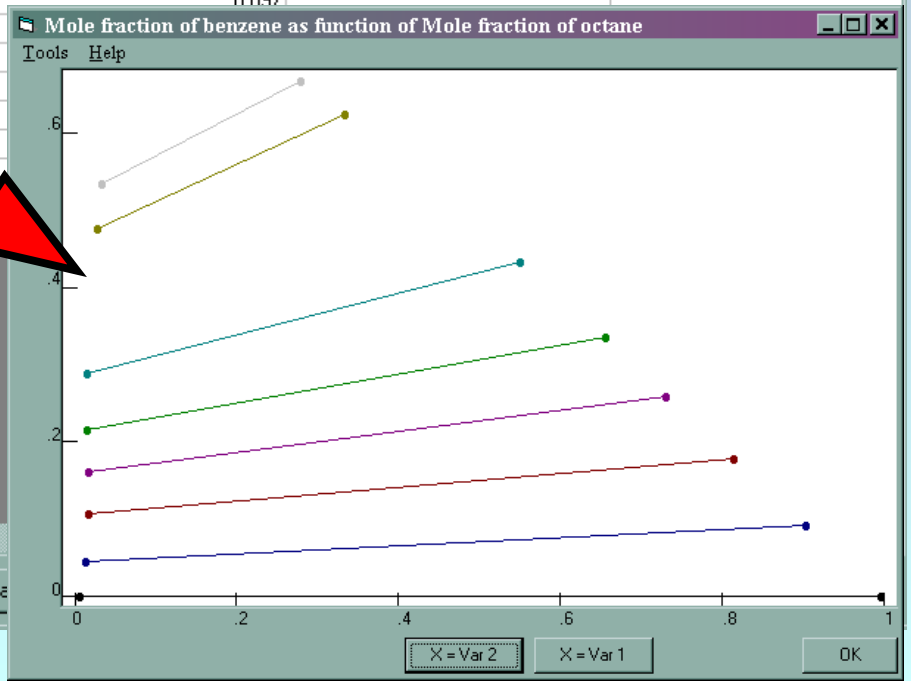
Property	Temperature	Mole fraction of octane	Mole fraction of benzene	Mole fraction of octane	Mole fraction of benzene
Units	K	Dimensionless	Dimensionless	Dimensionless	Dimensionless
Phase					
1	323.15	0.997	0.000	0.006	0.000
2	323.15	0.905	0.091	0.013	0.045
3	323.15	0.815	0.178	0.017	0.106
4	323.15	0.732	0.259	0.017	0.162
5	323.15	0.657	0.336	0.016	0.216
6	323.15	0.550	0.434	0.016	0.289
7	323.15	0.335	0.625	0.028	0.477
8	323.15	0.279	0.668	0.034	0.535
9					
19	373.15	0.812	0.173	0.015	0.097
20	373.15	0.720	0.259	0.015	
21	373.15	0.646		0.028	
22	373.15	0.476		0.032	
23	373.15	0.399	0.532	0.050	
24	373.15	0.300	0.598	0.057	
25					

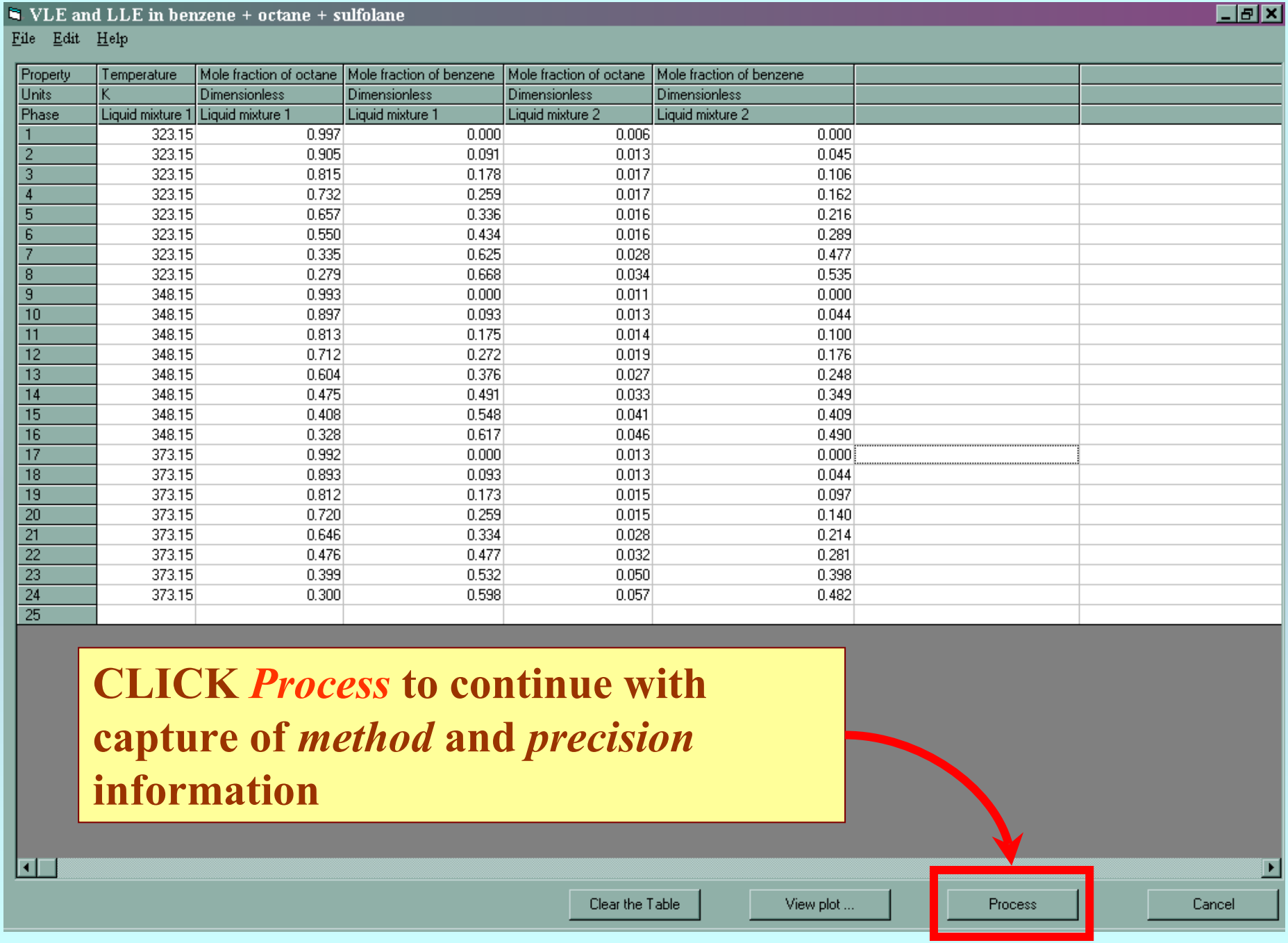
NOTE: You can *SELECT* the data that you wish to plot.
This can make the plot easier to interpret.
1) SELECT data **2)** CLICK View plot

Clear the Ta

Mole fraction of benzene as function of Mole fraction of octane

Tools Help

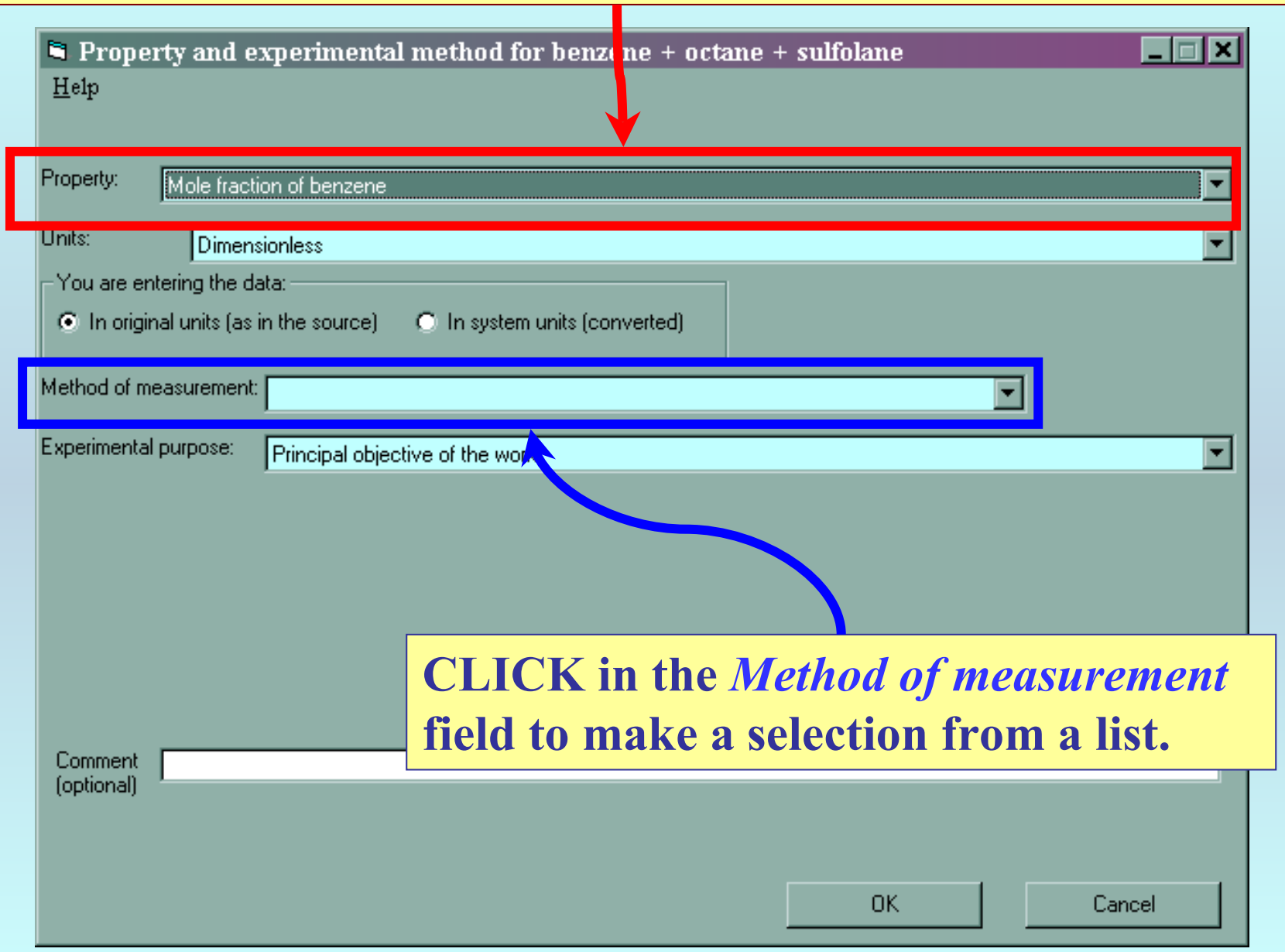



VLE and LLE in benzene + octane + sulfolane
File Edit Help
Property | Temperature | Mole fraction of octane | Mole fraction of benzene | Mole fraction of octane | Mole fraction of benzene
Units | K | Dimensionless | Dimensionless | Dimensionless | Dimensionless
Phase | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 1 | Liquid mixture 2 | Liquid mixture 2
1 | 323.15 | 0.997 | 0.000 | 0.006 | 0.000
2 | 323.15 | 0.905 | 0.091 | 0.013 | 0.045
3 | 323.15 | 0.815 | 0.178 | 0.017 | 0.106
4 | 323.15 | 0.732 | 0.259 | 0.017 | 0.162
5 | 323.15 | 0.657 | 0.336 | 0.016 | 0.216
6 | 323.15 | 0.550 | 0.434 | 0.016 | 0.289
7 | 323.15 | 0.335 | 0.625 | 0.028 | 0.477
8 | 323.15 | 0.279 | 0.668 | 0.034 | 0.535
9 | 348.15 | 0.993 | 0.000 | 0.011 | 0.000
10 | 348.15 | 0.897 | 0.093 | 0.013 | 0.044
11 | 348.15 | 0.813 | 0.175 | 0.014 | 0.100
12 | 348.15 | 0.712 | 0.272 | 0.019 | 0.176
13 | 348.15 | 0.604 | 0.376 | 0.027 | 0.248
14 | 348.15 | 0.475 | 0.491 | 0.033 | 0.349
15 | 348.15 | 0.408 | 0.548 | 0.041 | 0.409
16 | 348.15 | 0.328 | 0.617 | 0.046 | 0.490
17 | 373.15 | 0.992 | 0.000 | 0.013 | 0.000
18 | 373.15 | 0.893 | 0.093 | 0.013 | 0.044
19 | 373.15 | 0.812 | 0.173 | 0.015 | 0.097
20 | 373.15 | 0.720 | 0.259 | 0.015 | 0.140
21 | 373.15 | 0.646 | 0.334 | 0.028 | 0.214
22 | 373.15 | 0.476 | 0.477 | 0.032 | 0.281
23 | 373.15 | 0.399 | 0.532 | 0.050 | 0.398
24 | 373.15 | 0.300 | 0.598 | 0.057 | 0.482
25
CLICK Process to continue with capture of method and precision information
Clear the Table
View plot ...
Process
Cancel

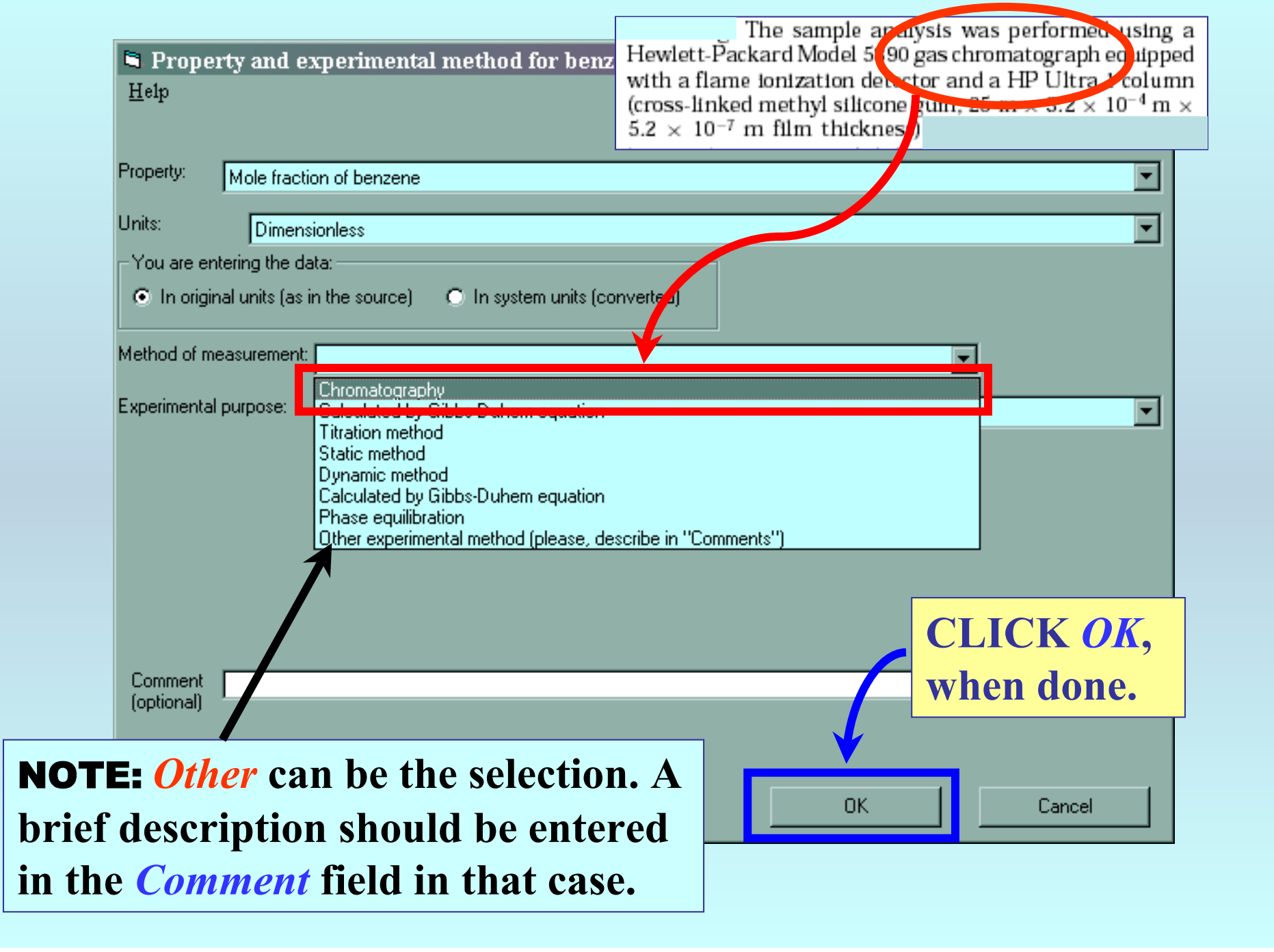
NOTE: **The GDC software *automatically* divides the entered table of LLE data into an appropriate number of separate data sets (*two in the present example*) based on the Gibbs Phase rule.**

The following screens capture information concerning the experimental methods and precisions for the data.

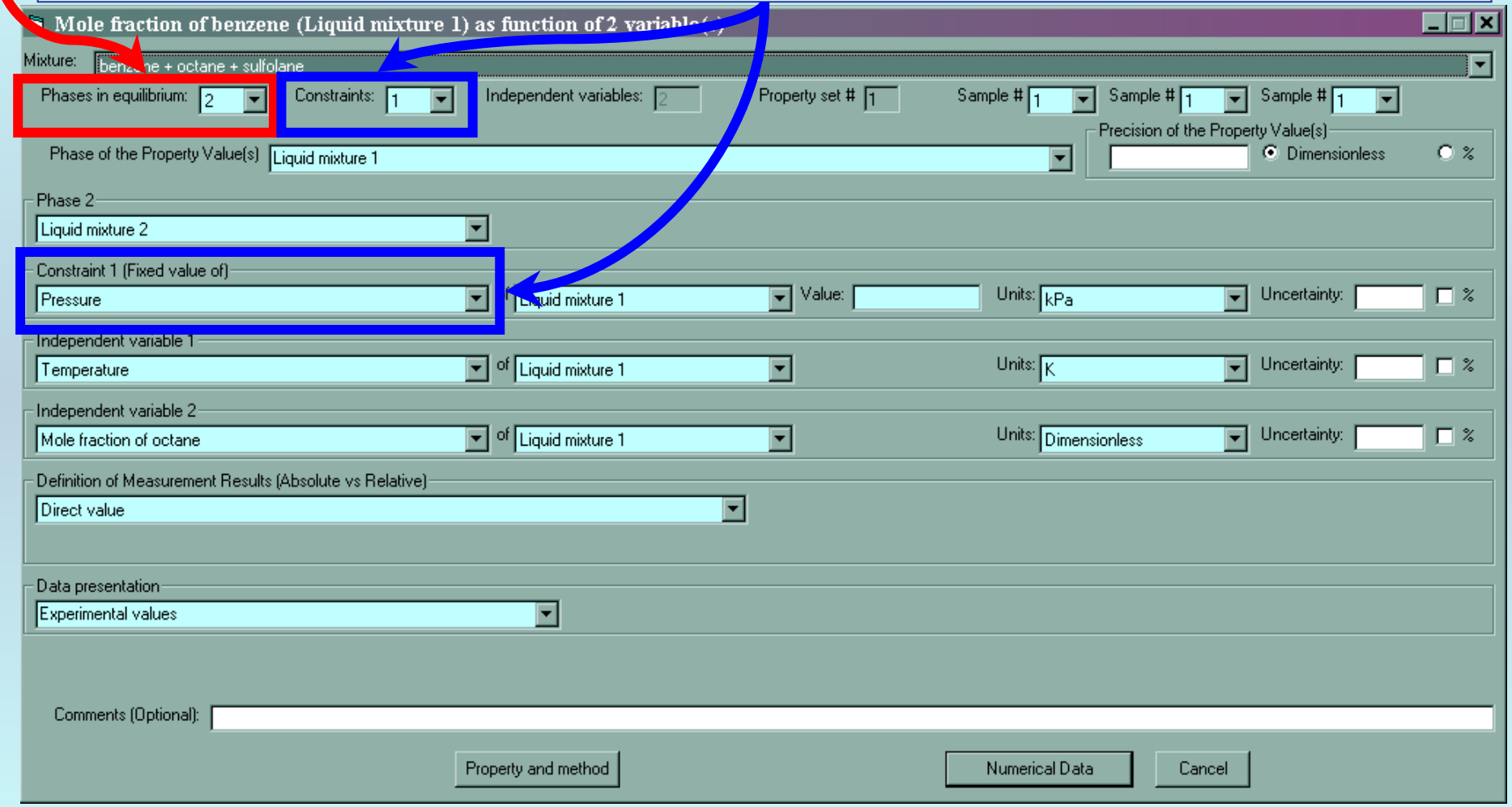
NOTE: The first *Property* is selected automatically by the software.



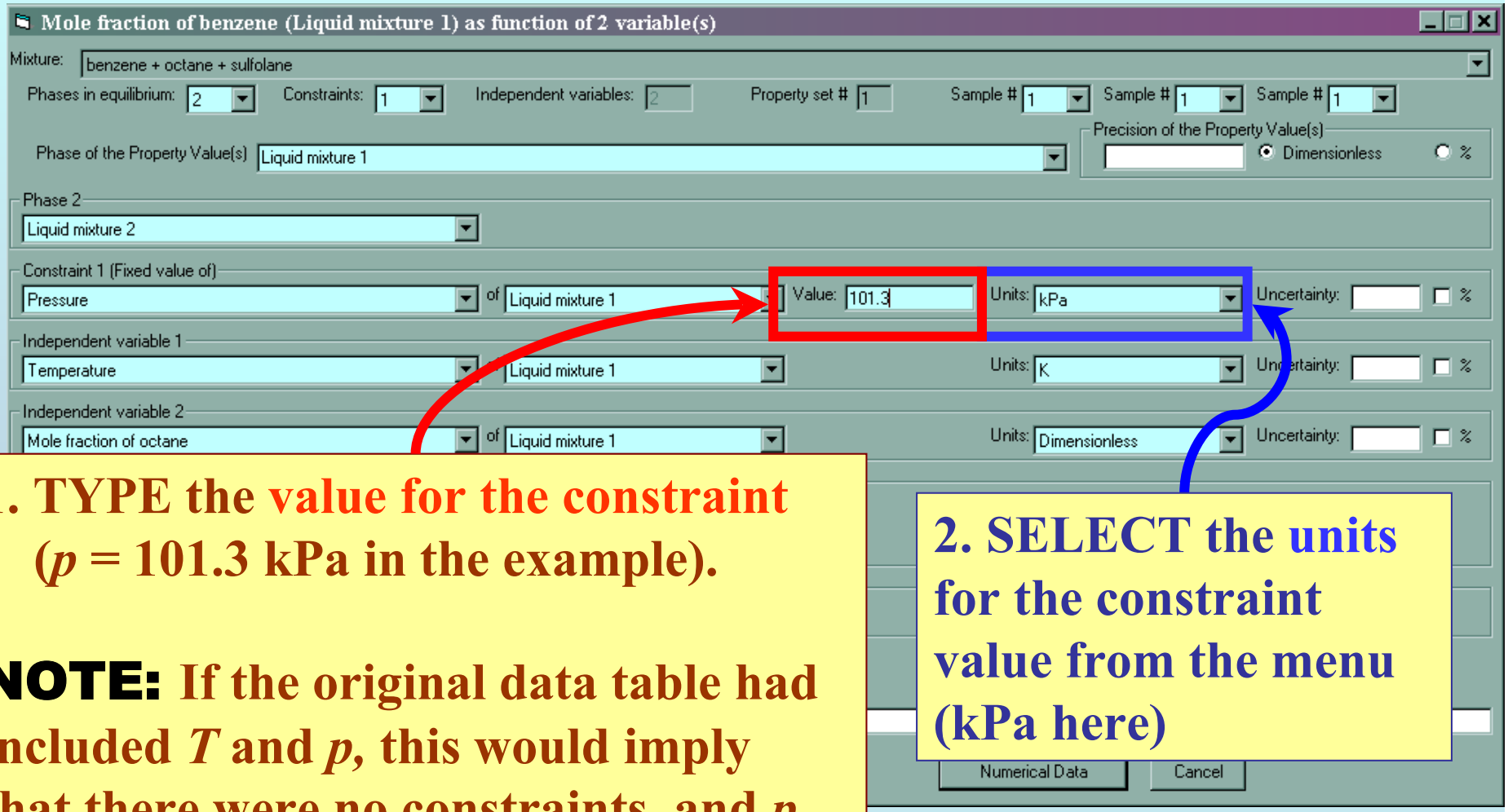
CLICK in the *Method of measurement* field to make a selection from a list.


The sample analysis was performed using a Hewlett-Packard Model 5890 gas chromatograph equipped with a flame ionization detector and a HP Ultra 1 column (cross-linked methyl silicone gum, 25 m × 3.2 × 10⁻⁴ m × 5.2 × 10⁻⁷ m film thickness)
Property and experimental method for benz
Help
Property:
Mole fraction of benzene
Units:
Dimensionless
You are entering the data:
In original units (as in the source)
In system units (converted)
Method of measurement:
Experimental purpose:
Chromatography
Titration method
Static method
Dynamic method
Calculated by Gibbs-Duhem equation
Phase equilibration
Other experimental method (please, describe in "Comments")
Comment (optional)
OK
Cancel
CLICK OK, when done.
NOTE: Other can be the selection. A brief description should be entered in the Comment field in that case.

NOTE: Based on the information pasted into the original table, the GDC software determines the # of *phases in equilibrium* and *contraints*. These fields are defined by the program.



Continue with the tutorial...



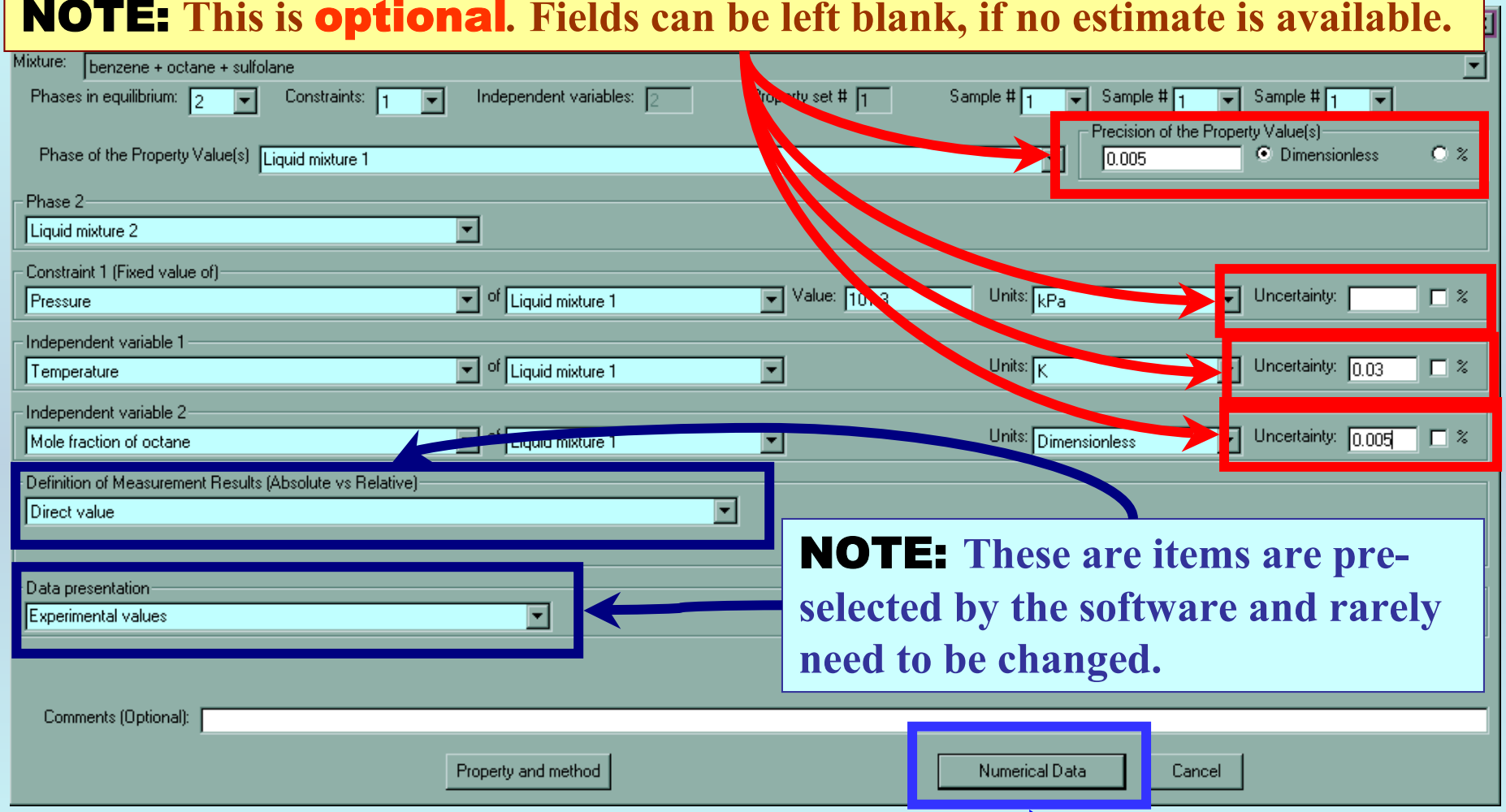
1. TYPE the value for the constraint (p = 101.3 kPa in the example).

NOTE: If the original data table had included T and p, this would imply that there were no constraints, and p would be listed as a variable here, also.

2. SELECT the units for the constraint value from the menu (kPa here)

1. TYPE estimated precisions for the *property*, *constraint(s)*, and *independent-variable value(s)*.

NOTE: This is optional. Fields can be left blank, if no estimate is available.



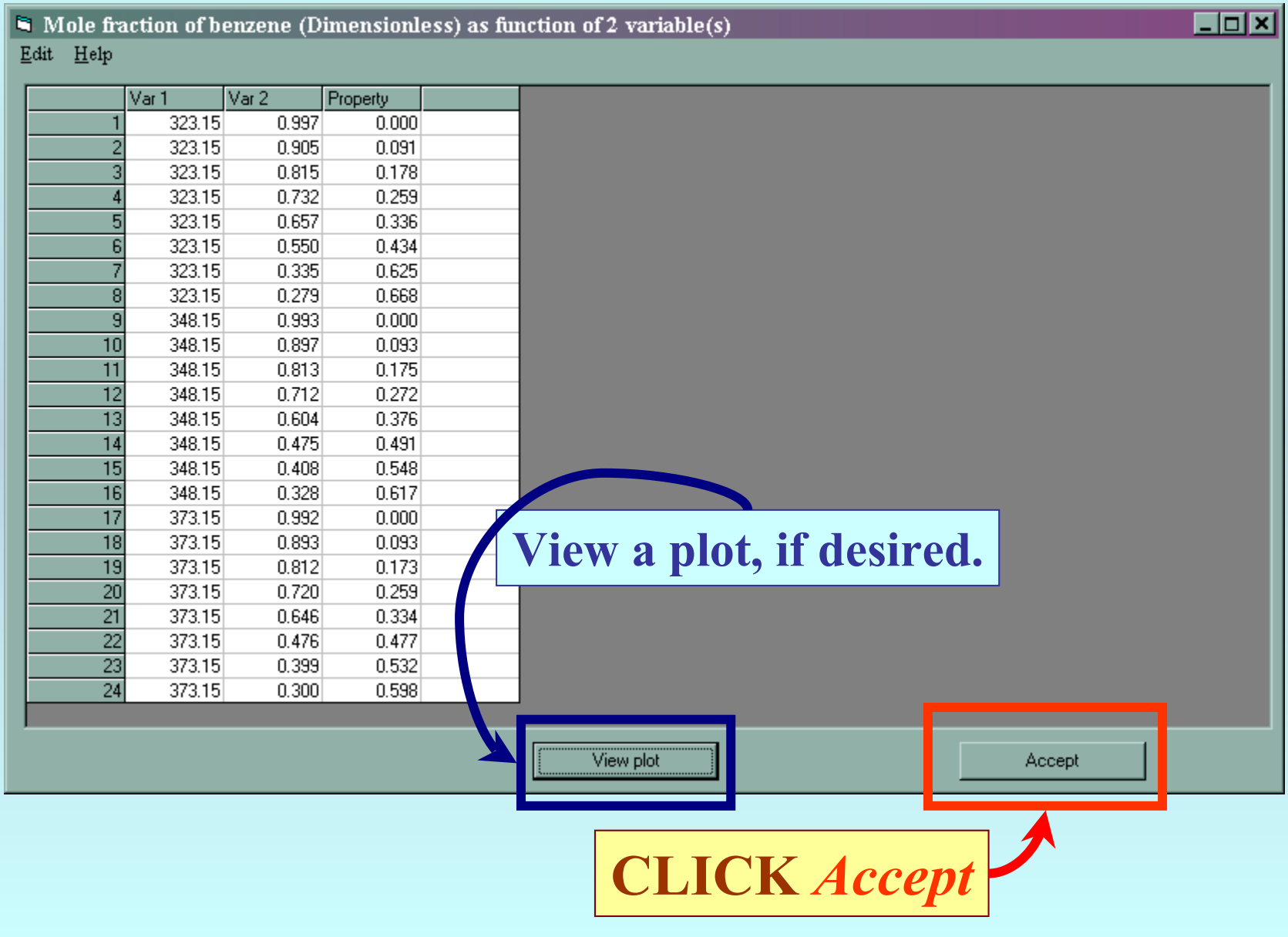
NOTE: These are items are pre-selected by the software and rarely need to be changed.

Recall...

Mass fraction measurements were reproducible to within ±0.005.

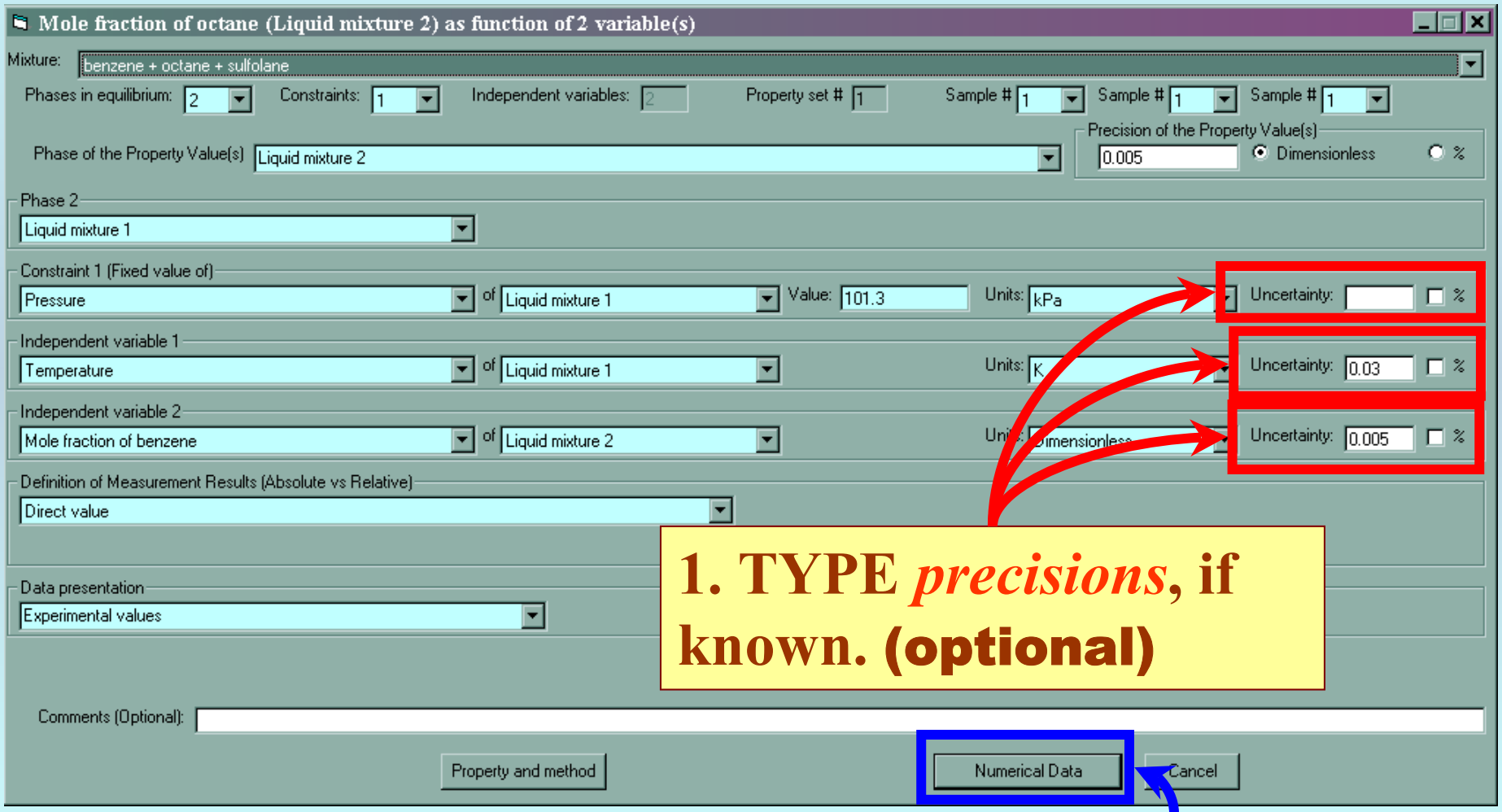
Temperatures were controlled to ±0.03 K.

2. CLICK *Numerical Data*


Mole fraction of benzene (Dimensionless) as function of 2 variable(s)
Edit
Help
Var 1
Var 2
Property
1 323.15 0.997 0.000
2 323.15 0.905 0.091
3 323.15 0.815 0.178
4 323.15 0.732 0.259
5 323.15 0.657 0.336
6 323.15 0.550 0.434
7 323.15 0.335 0.625
8 323.15 0.279 0.668
9 348.15 0.993 0.000
10 348.15 0.897 0.093
11 348.15 0.813 0.175
12 348.15 0.712 0.272
13 348.15 0.604 0.376
14 348.15 0.475 0.491
15 348.15 0.408 0.548
16 348.15 0.328 0.617
17 373.15 0.992 0.000
18 373.15 0.893 0.093
19 373.15 0.812 0.173
20 373.15 0.720 0.259
21 373.15 0.646 0.334
22 373.15 0.476 0.477
23 373.15 0.399 0.532
24 373.15 0.300 0.598
View a plot, if desired.
View plot
Accept
CLICK Accept

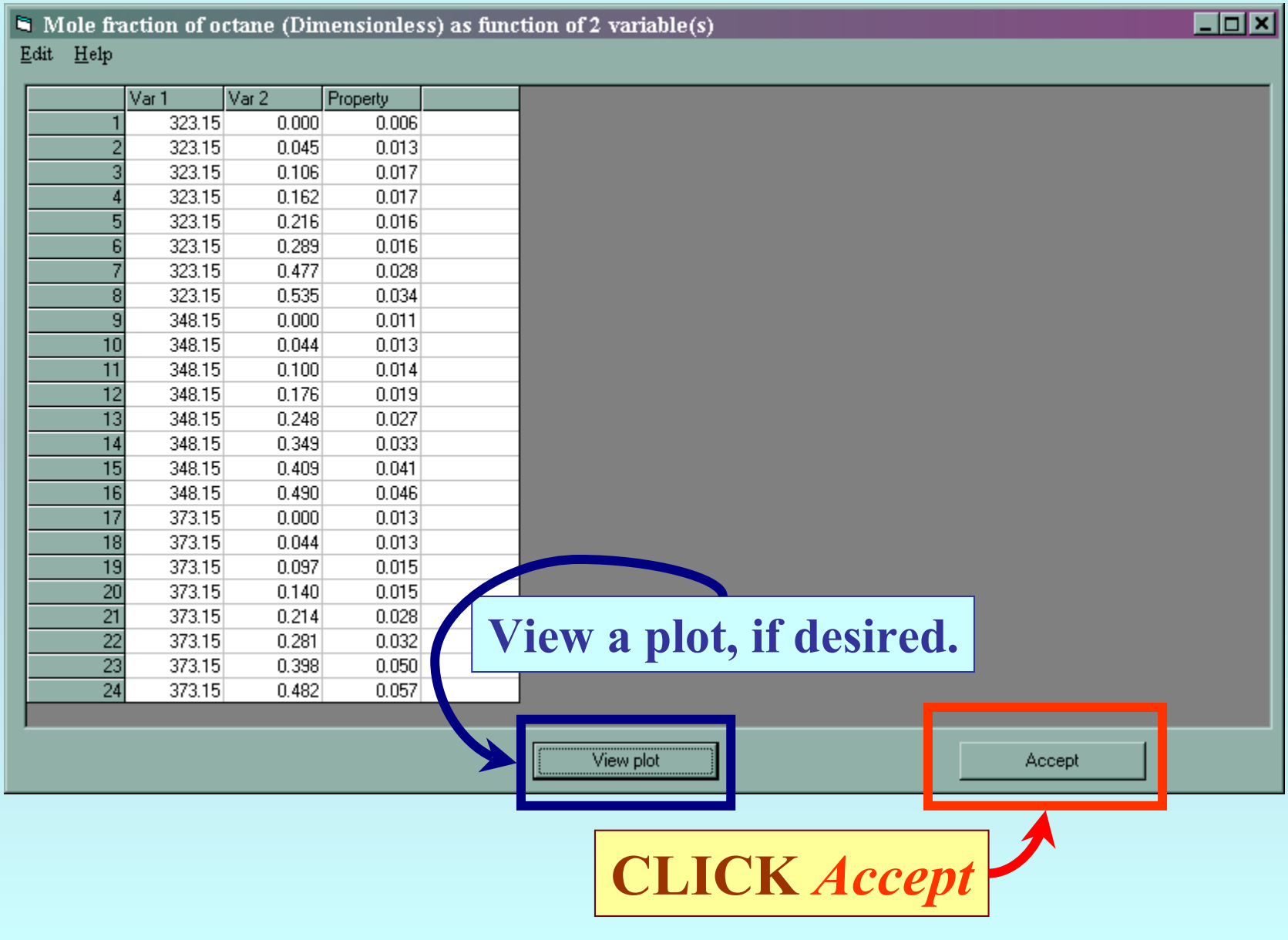
Continue with data capture for the second dataset obtained based upon the LLE data table.

NOTE: Most fields are filled automatically by the software.

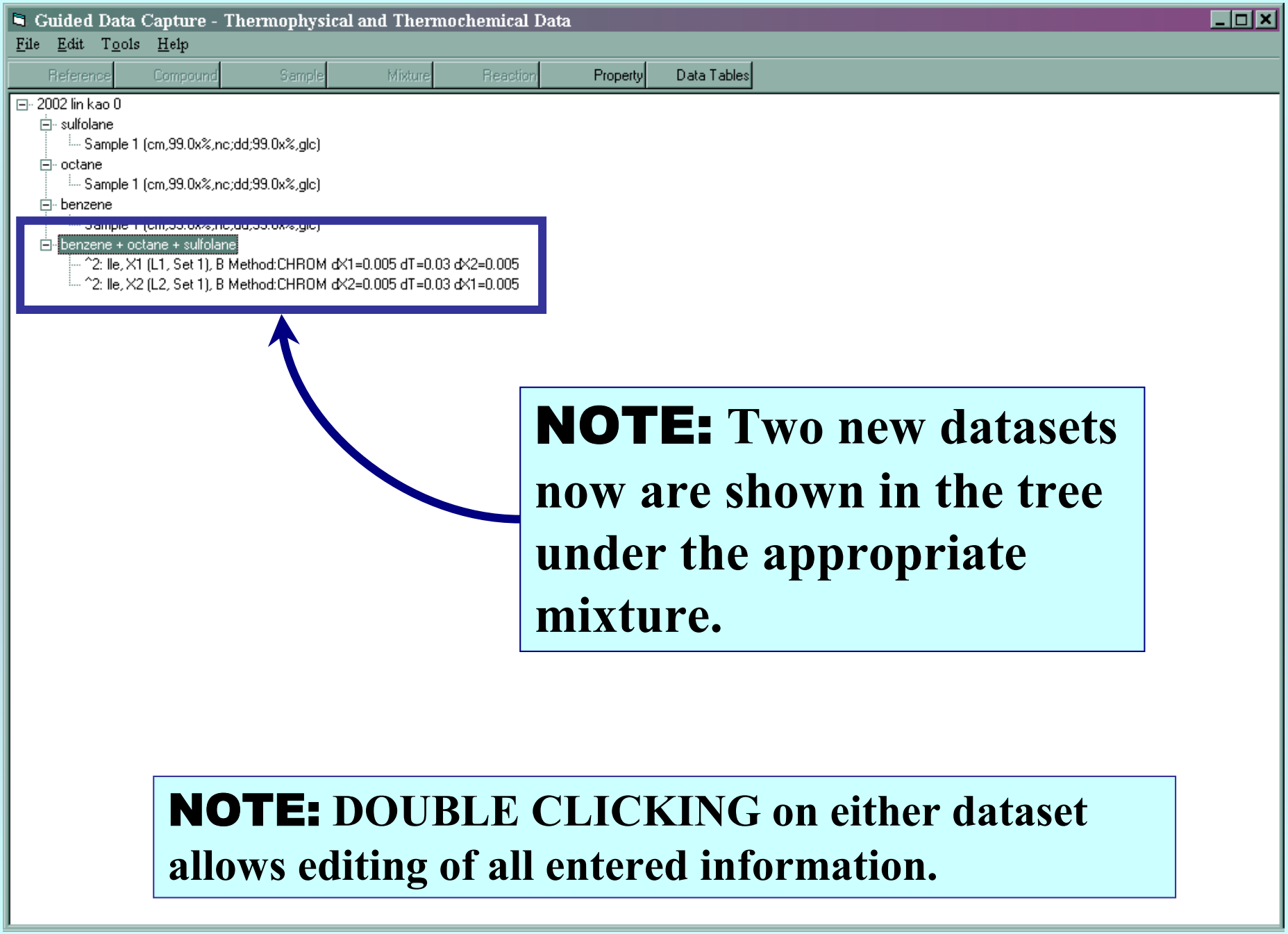


1. TYPE *precisions*, if known. (optional)

2. CLICK *Numerical Data*



	Var 1	Var 2	Property
1	323.15	0.000	0.006
2	323.15	0.045	0.013
3	323.15	0.106	0.017
4	323.15	0.162	0.017
5	323.15	0.216	0.016
6	323.15	0.289	0.016
7	323.15	0.477	0.028
8	323.15	0.535	0.034
9	348.15	0.000	0.011
10	348.15	0.044	0.013
11	348.15	0.100	0.014
12	348.15	0.176	0.019
13	348.15	0.248	0.027
14	348.15	0.349	0.033
15	348.15	0.409	0.041
16	348.15	0.490	0.046
17	373.15	0.000	0.013
18	373.15	0.044	0.013
19	373.15	0.097	0.015
20	373.15	0.140	0.015
21	373.15	0.214	0.028
22	373.15	0.281	0.032
23	373.15	0.398	0.050
24	373.15	0.482	0.057



NOTE: Two new datasets now are shown in the tree under the appropriate mixture.

NOTE: DOUBLE CLICKING on either dataset allows editing of all entered information.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program.**