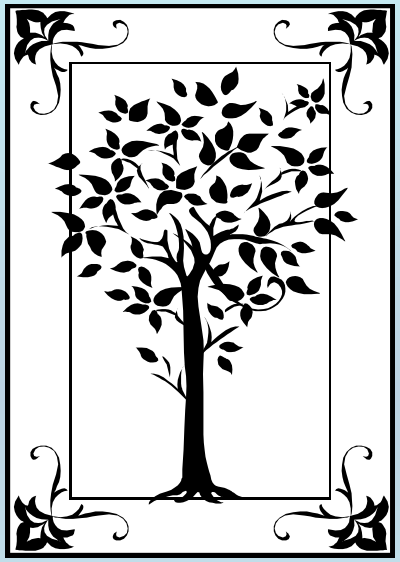
METADATA AND NUMERICAL DATA CAPTURE:
Binary Diffusion Coefficient
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for Binary Diffusion Coefficient
(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:

4462 *Ind. Eng. Chem. Res.* 2000, *39,* 4462−4469

Measurements of Binary Diffusion Coefficients and Partition Ratios for Acetone, Phenol, α-Tocopherol, and β-Carotene in Supercritical Carbon Dioxide with a Poly(ethylene glycol)-Coated Capillary Column

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Binary diffusion coefficients, D_{12}, and partition ratios, k, for the poly(ethylene glycol) (PEG) layer to supercritical carbon dioxide for acetone and some solid solutes such as phenol, α-tocopherol, and β-carotene were measured with a PEG-coated capillary column by a tracer response technique. The D_{12} values for acetone with the PEG-coated column were consistent with those measured by the Taylor dispersion method in which an uncoated capillary column was employed. The D_{12} and k values for all of the solutes decrease simply with increasing pressure, and the D_{12} values were represented by the Schmidt number correlation.

Binary Diffusion Coefficients for α-tocopherol in CO_2 (supercritical) at various temperatures

Table 3. Measured Binary Diffusion Coefficients D_{12} and Partition Ratios K for α-Tocopherol and β-Carotene in Supercritical Carbon Dioxide at 313.15 and 323.15 K

tracer	T (K)	P (MPa)	D_{12} (10^{-8} m^2/s)	k	
α-tocopherol	313.15	12.16	0.704	1.057	9
		12.20	0.698	1.021	7
		13.33	0.670	0.789	6
		14.30	0.649	0.668	7.05E−03
		15.25	0.631	0.584	4.90E−03
		16.17	0.629	0.534	5.74E−03
		16.18	0.605	0.527	1.34E−02
		16.20	0.607	0.526	8.69E−03
		17.04	0.619	0.485	3.18E−03
		17.73	0.599	0.448	4.17E−03
		18.02	0.586	0.435	7.03E−03
		18.91	0.583	0.406	4.22E−03
		19.63	0.573	0.384	3.99E−03
		20.03	0.563	0.369	4.66E−03
		21.47	0.541	0.339	3.96E−03
		21.95	0.517	0.311	3.74E−03
		23.05	0.522	0.301	4.60E−03
	323.15	16.05	0.729	0.719	8.02E−03
		18.05	0.690	0.518	5.52E−03
		20.08	0.661	0.410	4.66E−03
		22.07	0.621	0.336	2.88E−03

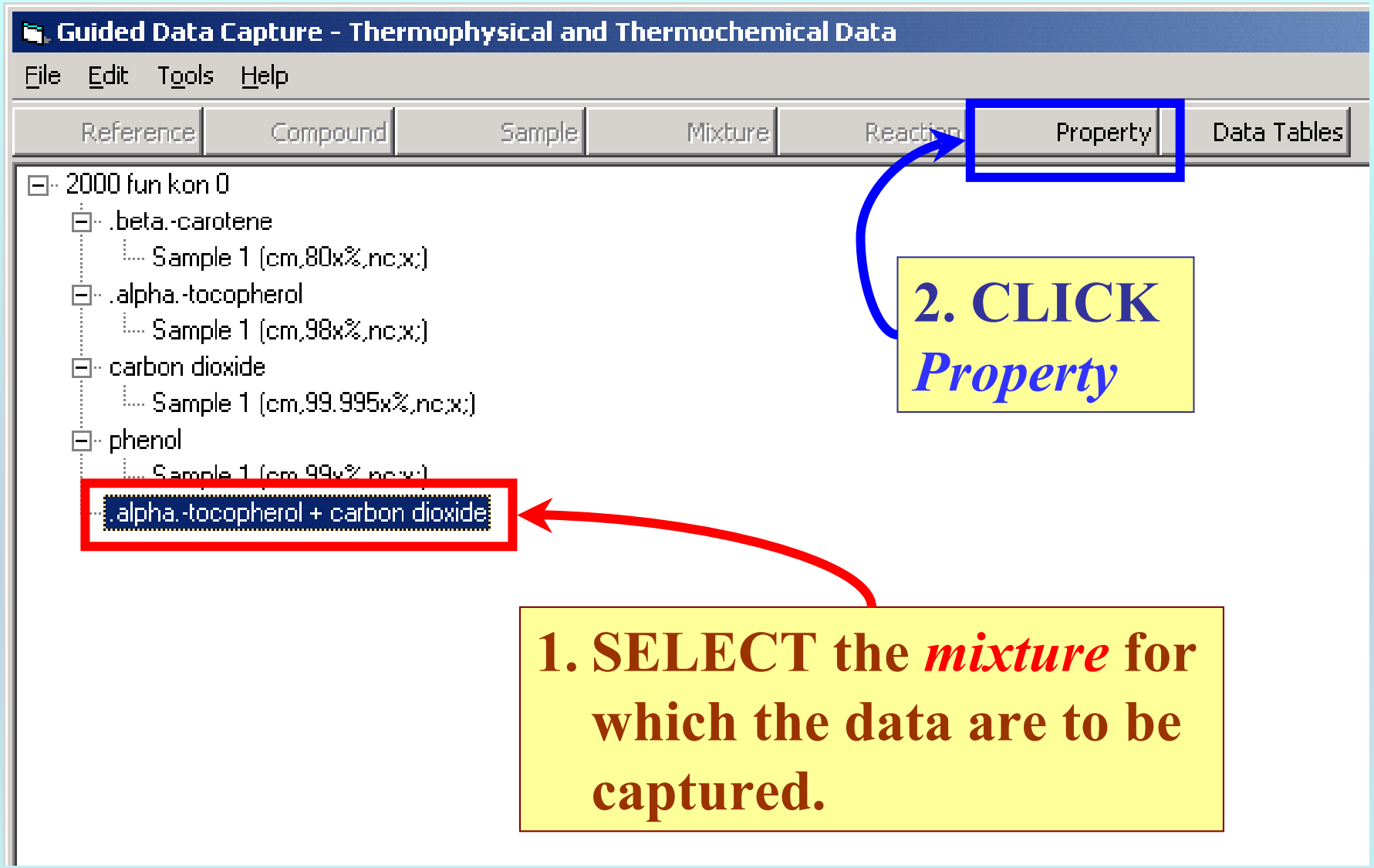
This data set is considered here.

Experimental Method Info:

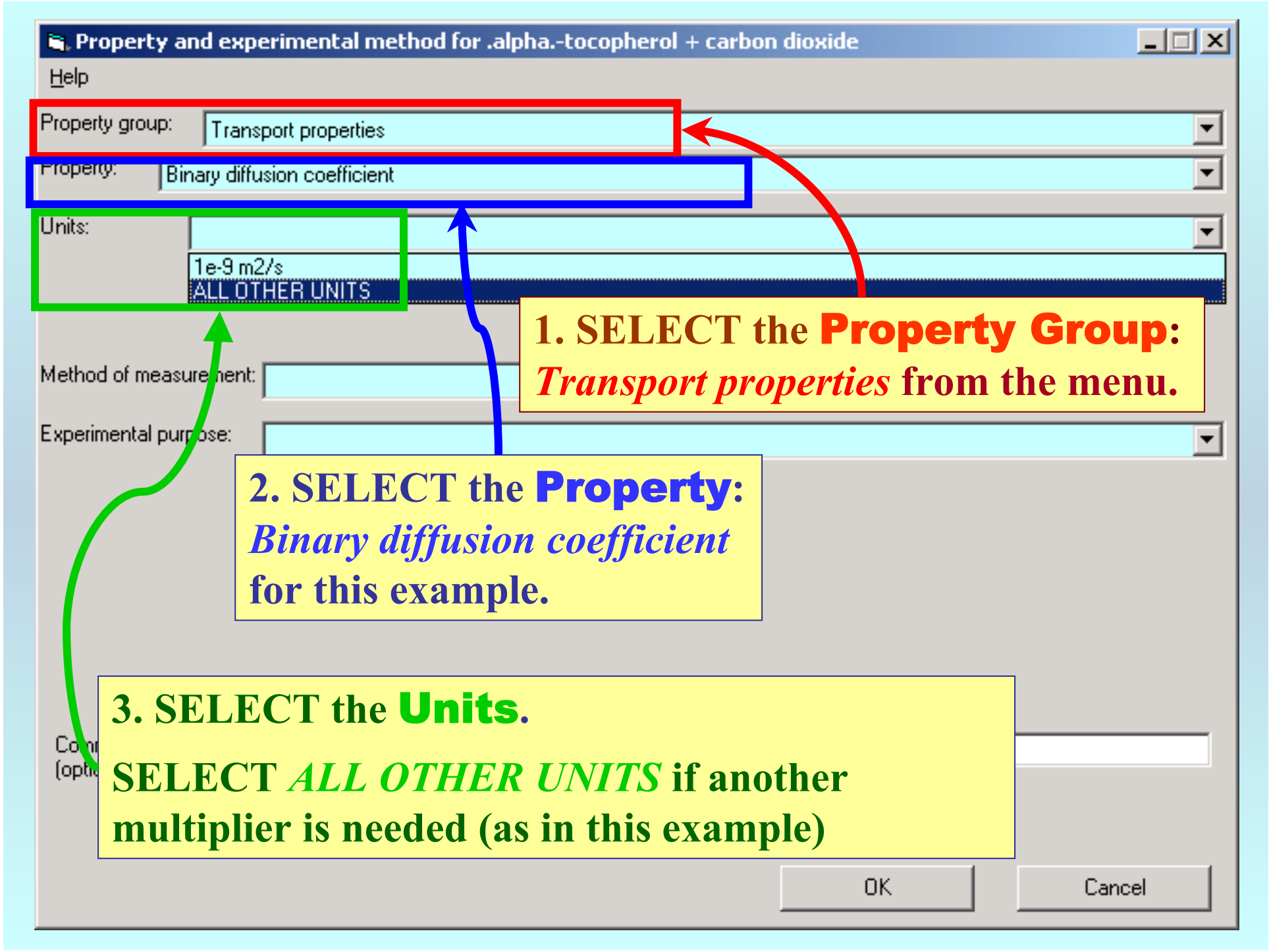
Method: Taylor Dispersion (Tracer response technique)

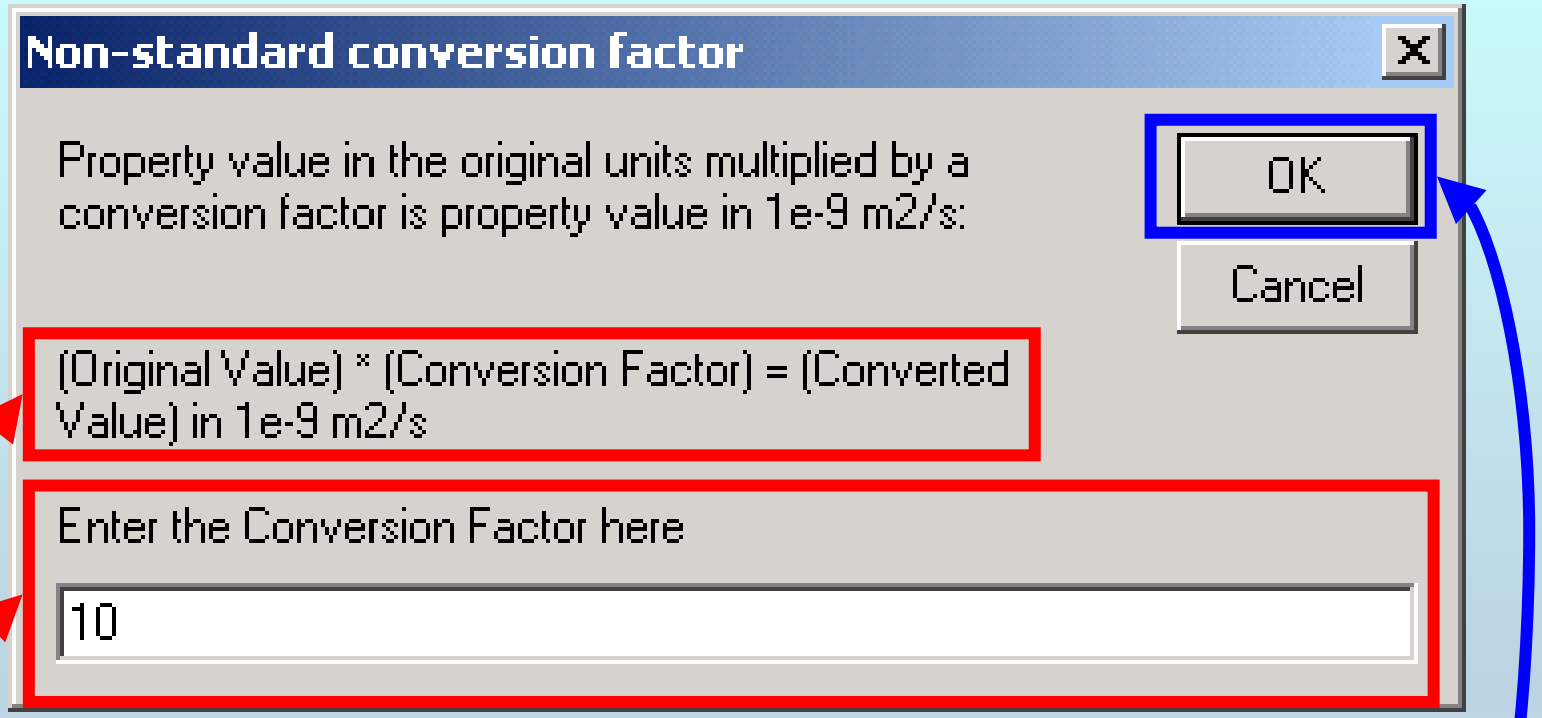
Uncertainty Info:

Figure 9 shows the Schmidt number correlations[26,40] for acetone, α-tocopherol, and β-carotene. It is found that the D_{12} values for acetone are well correlated, and those for α-tocopherol (AAD% = 10.7, N = 22) and β-carotene (AAD% = 6.5, N = 21) are substantially predictable with this correlation.



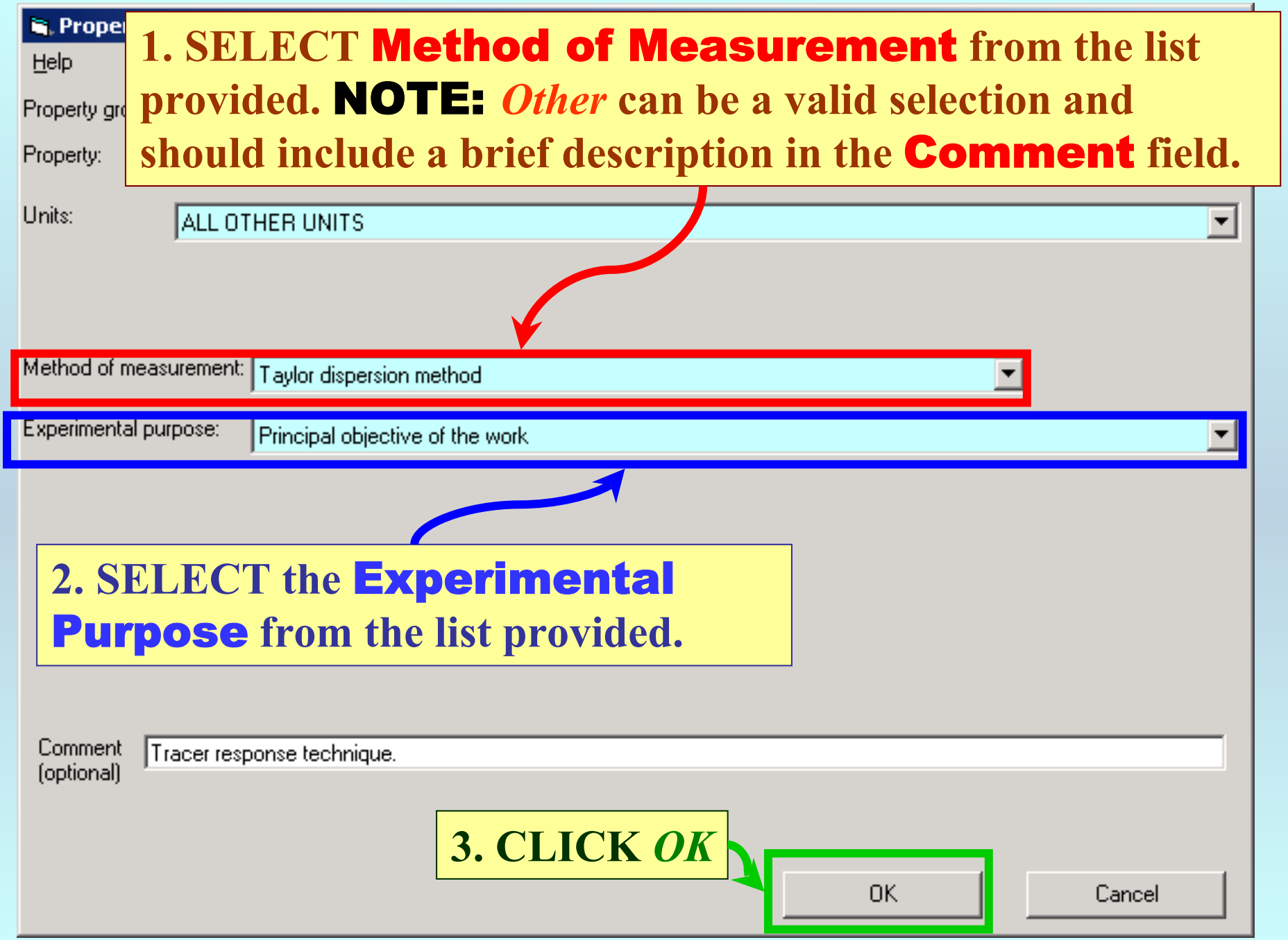
NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for .alpha.-tocopherol + carbon dioxide
Help
Property group:
Transport properties
Property:
Binary diffusion coefficient
Units:
1e-9 m2/s
ALL OTHER UNITS
Method of measurement:
Experimental purpose:
1. SELECT the Property Group:
Transport properties from the menu.
2. SELECT the Property:
Binary diffusion coefficient
for this example.
3. SELECT the Units.
SELECT ALL OTHER UNITS if another
multiplier is needed (as in this example)
OK
Cancel



1. ENTER the appropriate *Conversion Factor* based on the given equation. For the example: *10*.

2. CLICK OK

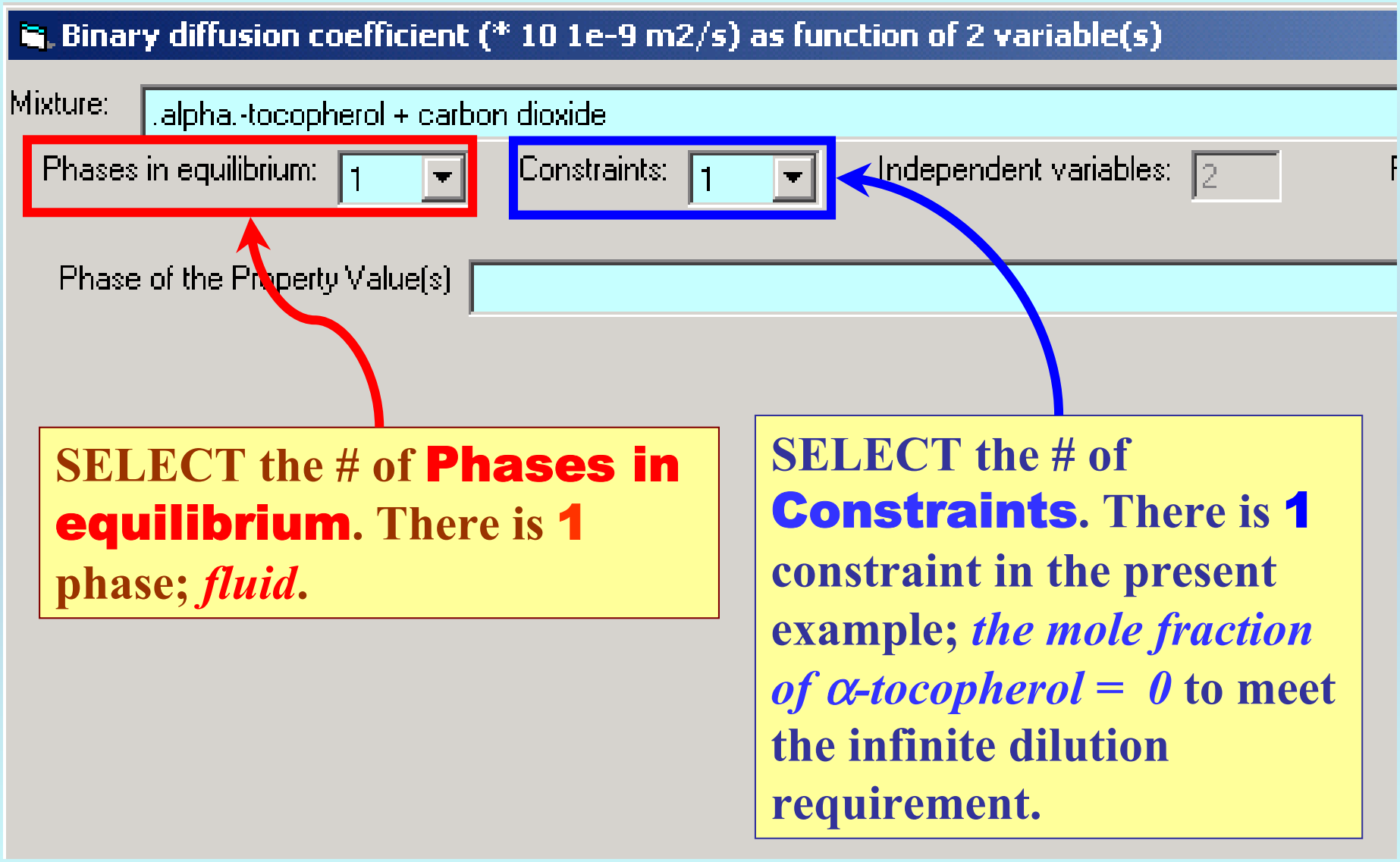


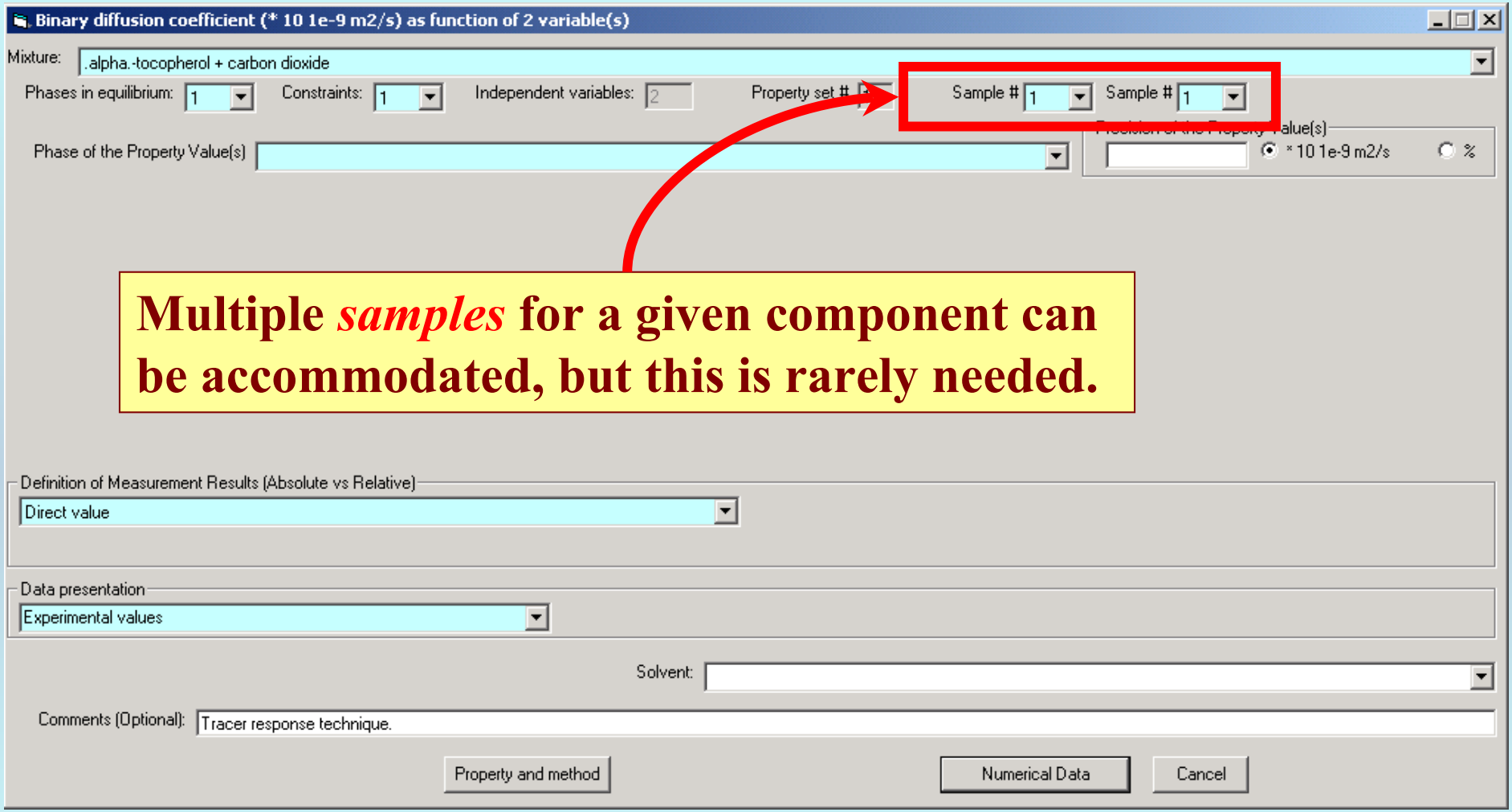
1. SELECT **Method of Measurement** from the list provided. **NOTE:** *Other* can be a valid selection and should include a brief description in the **Comment** field.

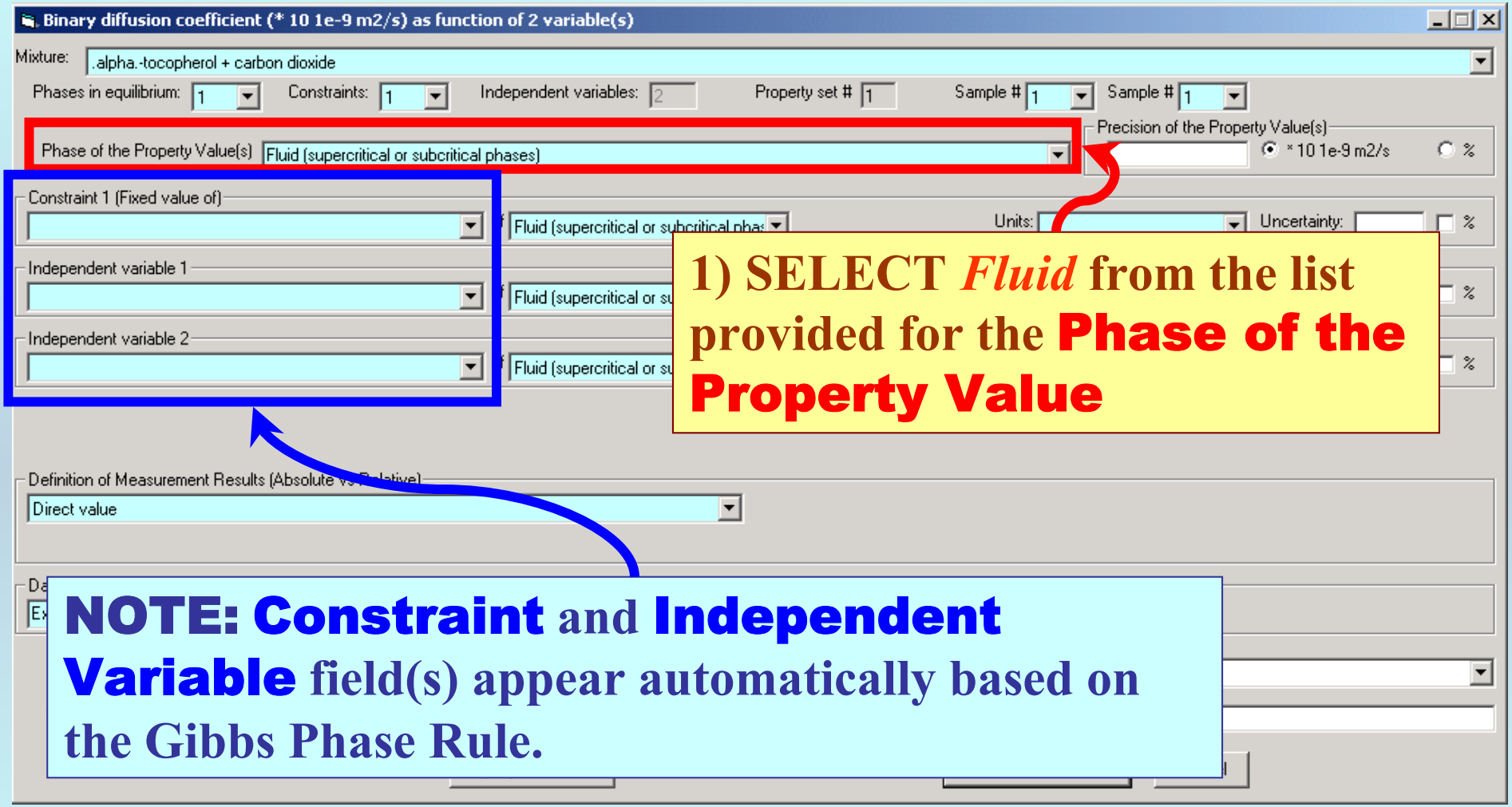
2. SELECT the **Experimental Purpose** from the list provided.

3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints

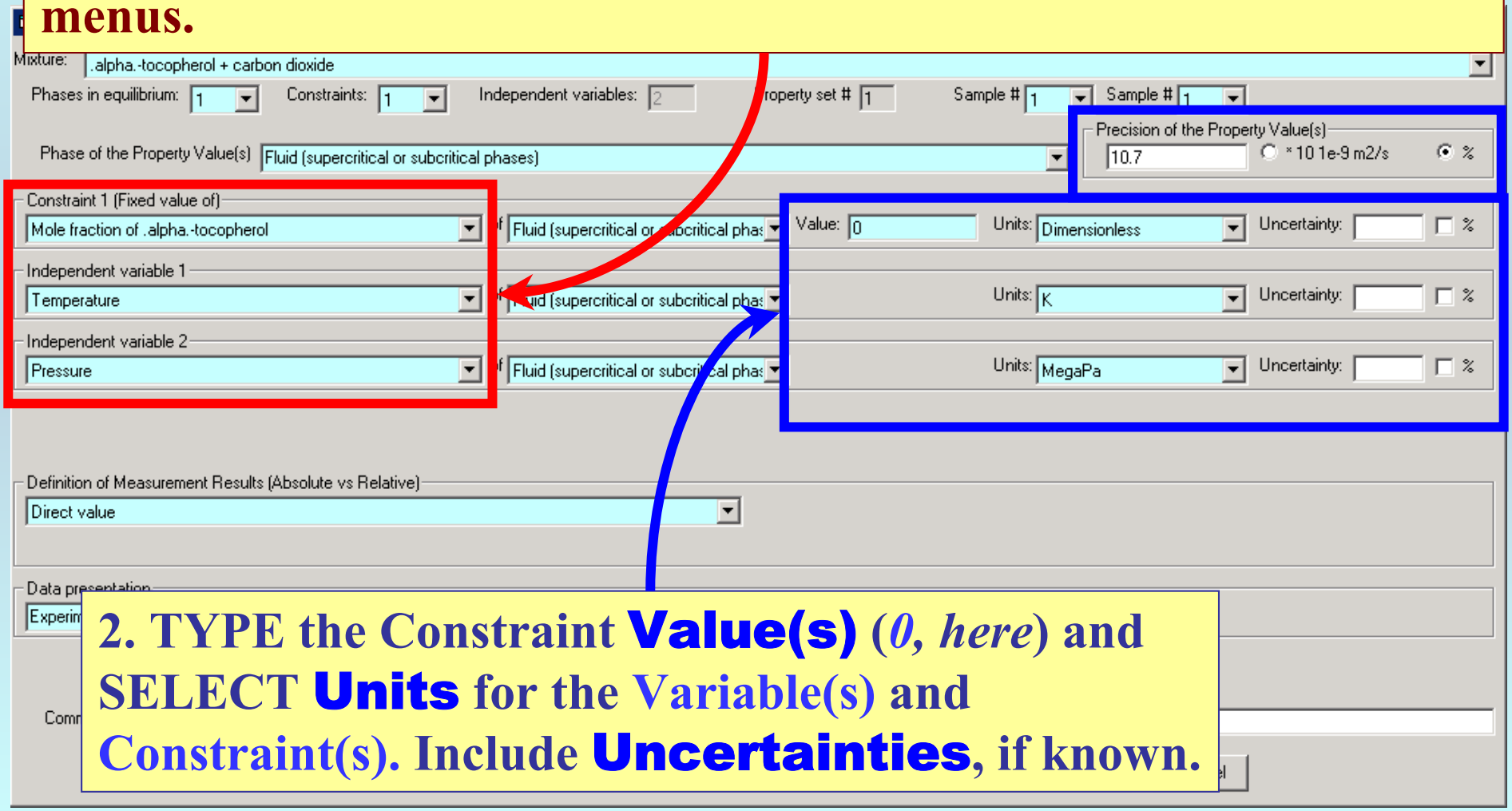



Binary diffusion coefficient (* 10 1e-9 m2/s) as function of 2 variable(s)
Mixture:
.alpha.-tocopherol + carbon dioxide
Phases in equilibrium:
1
Constraints:
1
Independent variables:
2
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
* 10 1e-9 m2/s
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Direct value
Data presentation
Experimental values
Solvent:
Comments (Optional):
Tracer response technique.
Property and method
Numerical Data
Cancel


Binary diffusion coefficient (* 10 1e-9 m2/s) as function of 2 variable(s)
Mixture: .alpha.-tocopherol + carbon dioxide
Phases in equilibrium: 1
Constraints: 1
Independent variables: 2
Property set # 1
Sample # 1
Sample # 1
Phase of the Property Value(s) Fluid (supercritical or subcritical phases)
Precision of the Property Value(s)
* 10 1e-9 m2/s
%
Constraint 1 (Fixed value of)
Units:
Uncertainty:
Independent variable 1
Independent variable 2
Definition of Measurement Results (Absolute vs. Relative)
Direct value
1) SELECT Fluid 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.

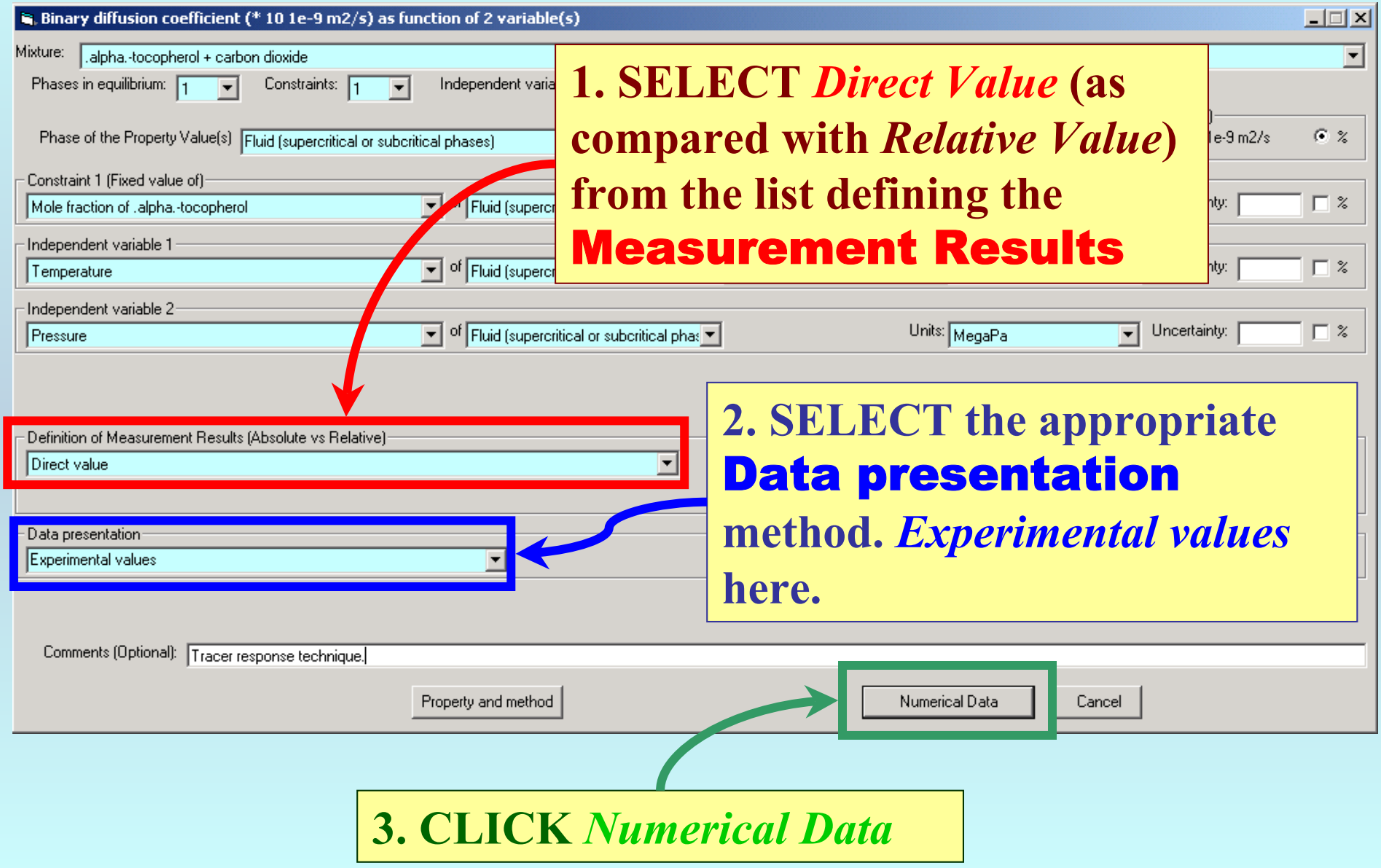
Specification of constraints, constraint values, and constraint units

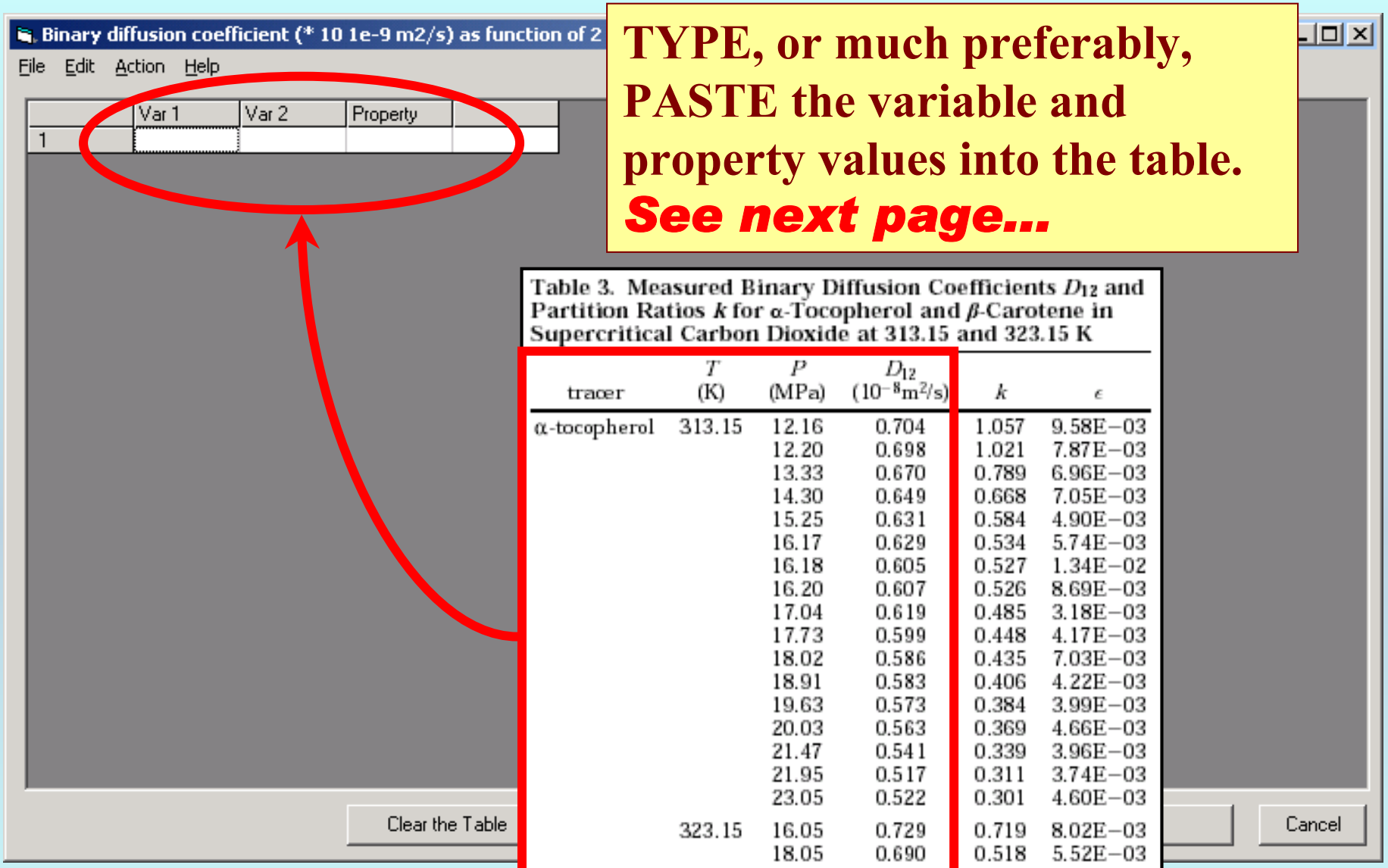
1. SELECT the Constraint(s) (*Mole fraction of α-tocopherol*) and the Independent Variable(s) (*T* and *p*, here) from the menus.



2. TYPE the Constraint Value(s) (*0, here*) 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. Measured Binary Diffusion Coefficients D_{12} and Partition Ratios k for α-Tocopherol and β-Carotene in Supercritical Carbon Dioxide at 313.15 and 323.15 K

tracer	T (K)	P (MPa)	D_{12} (10^{-8} m^2/s)	k	ϵ
α-tocopherol	313.15	12.16	0.704	1.057	9.58E−03
		12.20	0.698	1.021	7.87E−03
		13.33	0.670	0.789	6.96E−03
		14.30	0.649	0.668	7.05E−03
		15.25	0.631	0.584	4.90E−03
		16.17	0.629	0.534	5.74E−03
		16.18	0.605	0.527	1.34E−02
		16.20	0.607	0.526	8.69E−03
		17.04	0.619	0.485	3.18E−03
		17.73	0.599	0.448	4.17E−03
		18.02	0.586	0.435	7.03E−03
		18.91	0.583	0.406	4.22E−03
		19.63	0.573	0.384	3.99E−03
		20.03	0.563	0.369	4.66E−03
		21.47	0.541	0.339	3.96E−03
		21.95	0.517	0.311	3.74E−03
		23.05	0.522	0.301	4.60E−03
	323.15	16.05	0.729	0.719	8.02E−03
		18.05	0.690	0.518	5.52E−03
		20.08	0.661	0.410	4.66E−03
		22.07	0.621	0.336	2.88E−03

Binary diffusion coefficient (* 10 1e-9 m2/s) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	313.15	12.16	0.704
2	313.15	12.20	0.698
3	313.15	13.33	0.670
4	313.15	14.30	0.649
5	313.15	15.25	0.631
6	313.15	16.17	0.629
7	313.15	16.18	0.605
8	313.15	16.20	0.607
9	313.15	17.04	0.619
10	313.15	17.73	0.599
11	313.15	18.02	0.586
12	313.15	18.91	0.583
13	313.15	19.63	0.573
14	313.15	20.03	0.563
15	313.15	21.47	0.541
16	313.15	21.95	0.517
17	313.15	23.05	0.522
18	323.15	16.05	0.729
19	323.15	18.05	0.690
20	323.15	20.08	0.661
21	323.15	22.07	0.621

Clear the Table | View plot

Table 3. Measured Binary Diffusion Coefficients D_{12} and Partition Ratios k for α-Tocopherol and β-Carotene in Supercritical Carbon Dioxide at 313.15 and 323.15 K

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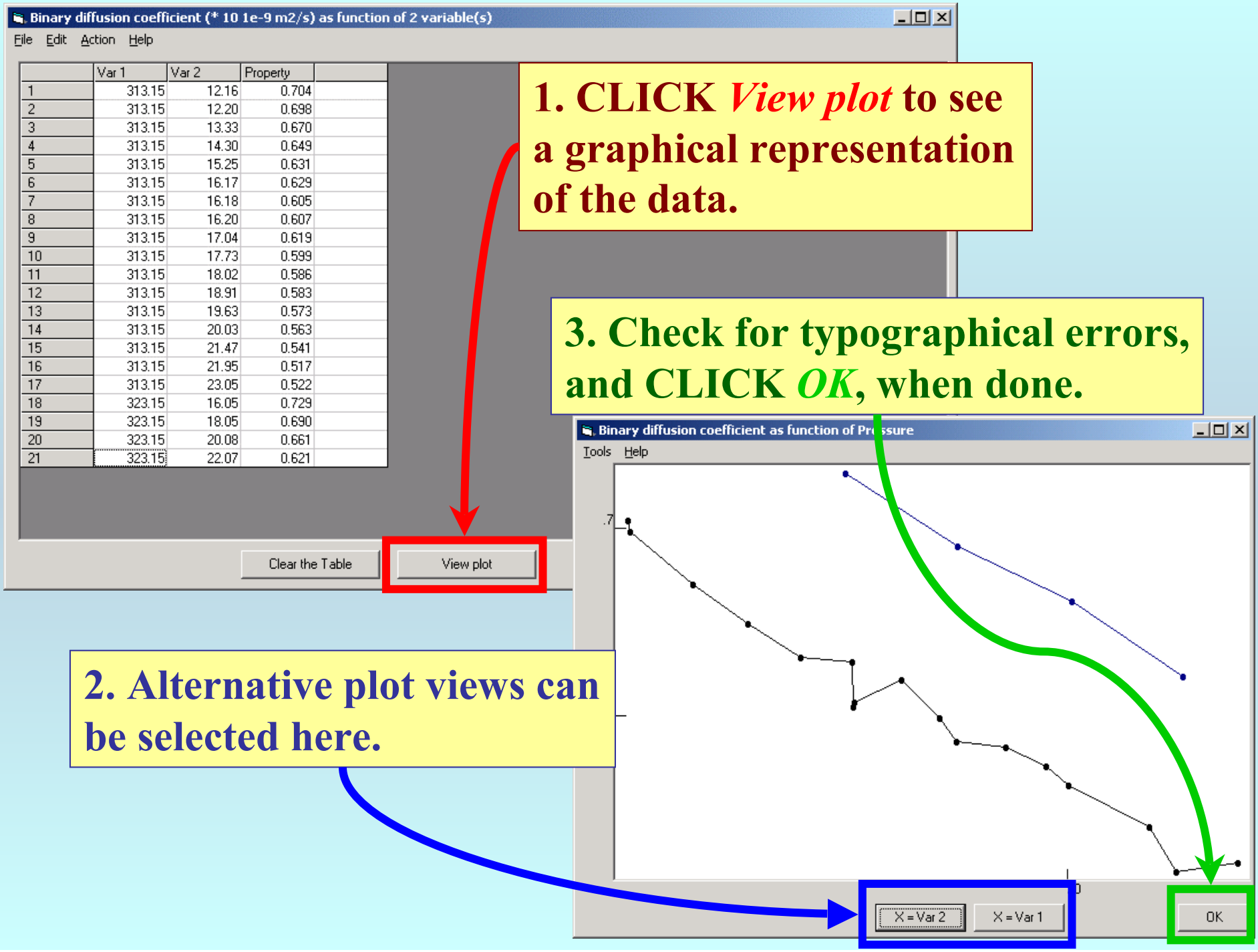
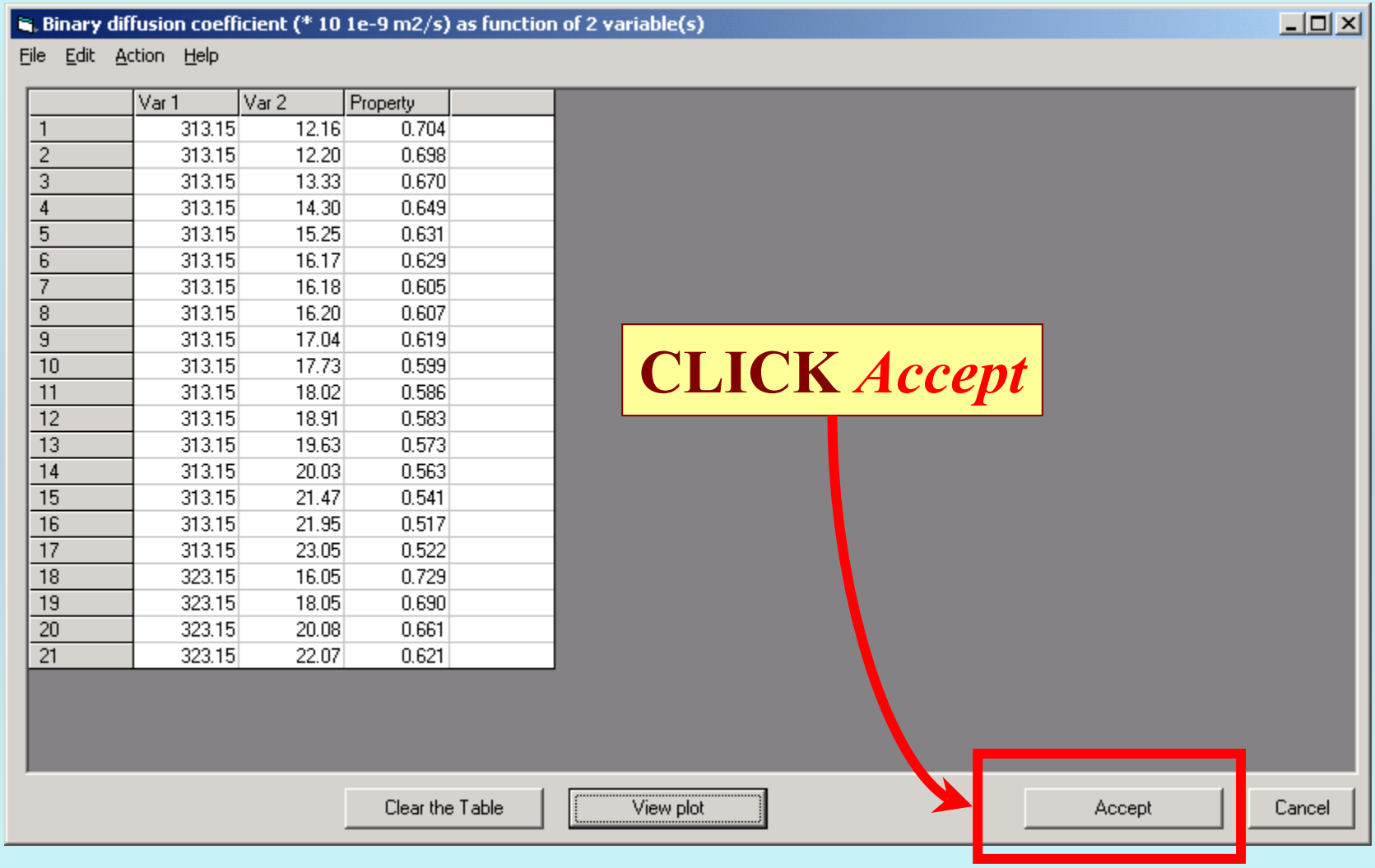
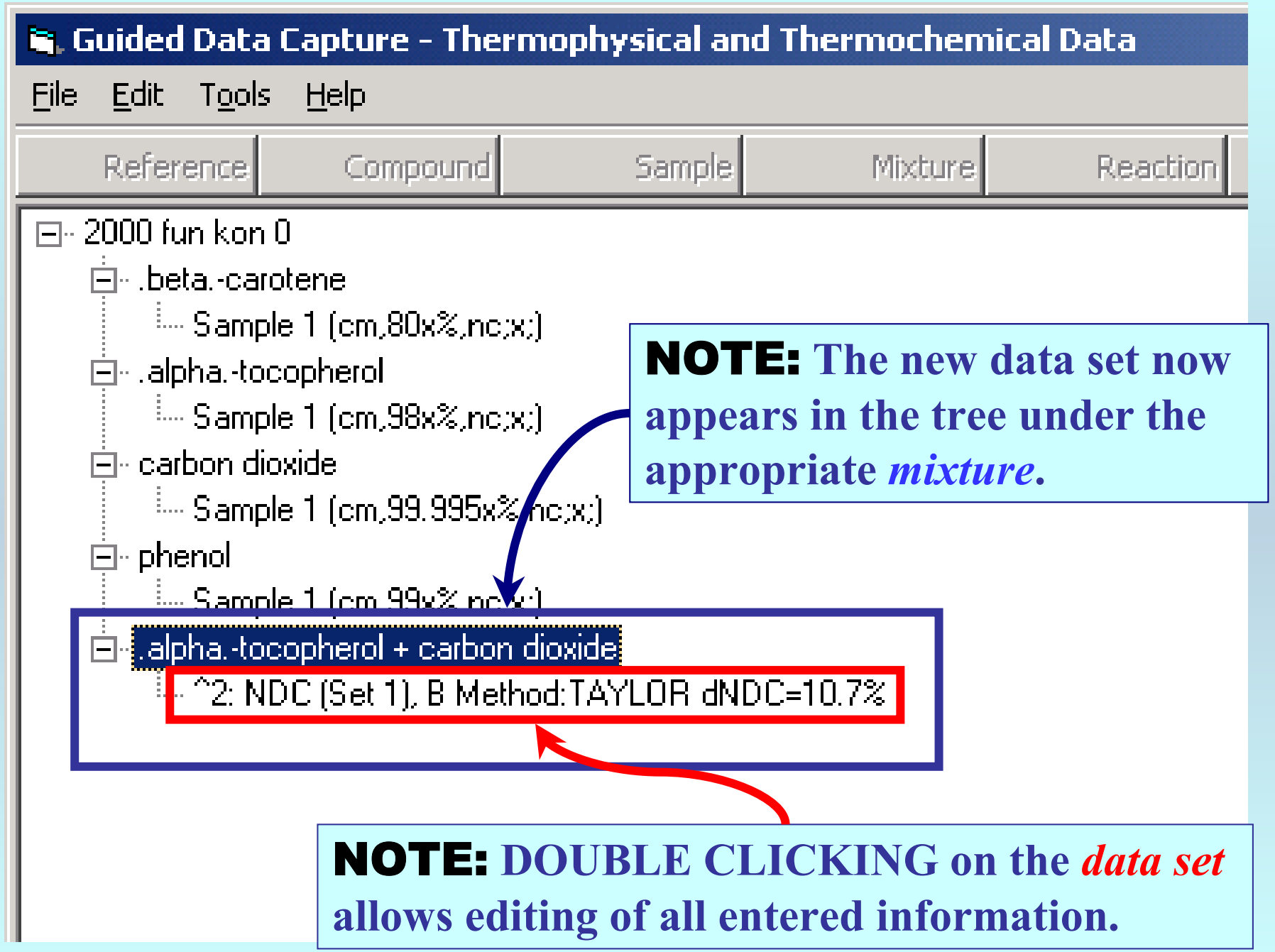
		20.08	0.661	0.410	4.66E−03
		22.07	0.621	0.336	2.88E−03

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.)


Binary diffusion coefficient (* 10 1e-9 m2/s) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 313.15 12.16 0.704
2 313.15 12.20 0.698
3 313.15 13.33 0.670
4 313.15 14.30 0.649
5 313.15 15.25 0.631
6 313.15 16.17 0.629
7 313.15 16.18 0.605
8 313.15 16.20 0.607
9 313.15 17.04 0.619
10 313.15 17.73 0.599
11 313.15 18.02 0.586
12 313.15 18.91 0.583
13 313.15 19.63 0.573
14 313.15 20.03 0.563
15 313.15 21.47 0.541
16 313.15 21.95 0.517
17 313.15 23.05 0.522
18 323.15 16.05 0.729
19 323.15 18.05 0.690
20 323.15 20.08 0.661
21 323.15 22.07 0.621
Clear the Table
View plot
1. CLICK View plot to see a graphical representation of the data.
3. Check for typographical errors, and CLICK OK, when done.
Binary diffusion coefficient as function of Pressure
Tools Help
X = Var 2
X = Var 1
OK
2. Alternative plot views can be selected here.


Binary diffusion coefficient (* 10 1e-9 m2/s) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 313.15 12.16 0.704
2 313.15 12.20 0.698
3 313.15 13.33 0.670
4 313.15 14.30 0.649
5 313.15 15.25 0.631
6 313.15 16.17 0.629
7 313.15 16.18 0.605
8 313.15 16.20 0.607
9 313.15 17.04 0.619
10 313.15 17.73 0.599
11 313.15 18.02 0.586
12 313.15 18.91 0.583
13 313.15 19.63 0.573
14 313.15 20.03 0.563
15 313.15 21.47 0.541
16 313.15 21.95 0.517
17 313.15 23.05 0.522
18 323.15 16.05 0.729
19 323.15 18.05 0.690
20 323.15 20.08 0.661
21 323.15 22.07 0.621
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
2000 fun kon 0
.beta.-carotene
Sample 1 (cm,80x%,nc;x;)
.alpha.-tocopherol
Sample 1 (cm,98x%,nc;x;)
carbon dioxide
Sample 1 (cm,99.995x%,nc;x;)
phenol
Sample 1 (cm,99x%,nc;x;)
.alpha.-tocopherol + carbon dioxide
^2: NDC (Set 1), B Method:TAYLOR dNDC=10.7%
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.**