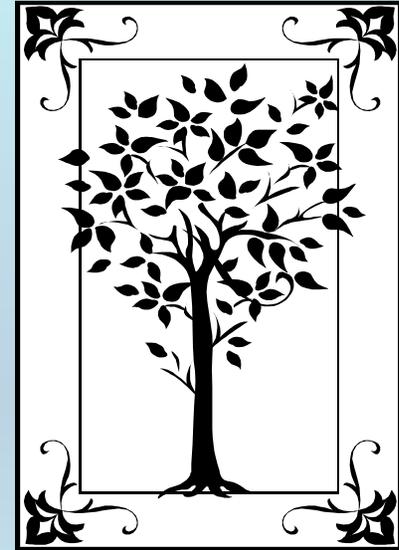


METADATA AND NUMERICAL DATA CAPTURE:
Binary Diffusion Coefficient
(2 – Components)

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} ($10^{-8}\text{m}^2/\text{s}$)	k
α -tocopherol	313.15	12.16	0.704	1.057
		12.20	0.698	1.021
		13.33	0.670	0.789
		14.30	0.649	0.668
		15.25	0.631	0.584
		16.17	0.629	0.534
		16.18	0.605	0.527
		16.20	0.607	0.526
		17.04	0.619	0.485
		17.73	0.599	0.448
		18.02	0.586	0.435
		18.91	0.583	0.406
		19.63	0.573	0.384
		20.03	0.563	0.369
		21.47	0.541	0.339
		21.95	0.517	0.311
		23.05	0.522	0.301
α -tocopherol	323.15	16.05	0.729	0.719
		18.05	0.690	0.518
		20.08	0.661	0.410
		22.07	0.621	0.336

**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.

The screenshot shows the 'Guided Data Capture - Thermophysical and Thermochemical Data' application. The interface includes a menu bar (File, Edit, Tools, Help) and a tabbed workspace with tabs for Reference, Compound, Sample, Mixture, Reaction, Property, and Data Tables. The 'Property' tab is highlighted with a blue box. A tree view on the left shows a hierarchy starting with '2000 fun kon 0', containing sub-items like '.beta.-carotene', '.alpha.-tocopherol', 'carbon dioxide', and 'phenol', each with a 'Sample 1' sub-entry. A red box highlights the entry 'alpha.-tocopherol + carbon dioxide' in the tree view, with a red arrow pointing to it from a yellow callout box. Another yellow callout box with a blue arrow points to the 'Property' tab.

2. CLICK *Property*

1. SELECT the *mixture* for which the data are to be captured.

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:

Count (opti)

OK Cancel

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)

Non-standard conversion factor [X]

Property value in the original units multiplied by a conversion factor is property value in 1 e-9 m²/s:

(Original Value) * (Conversion Factor) = (Converted Value) in 1 e-9 m²/s

Enter the Conversion Factor here

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.

Units: ALL OTHER UNITS

Method of measurement: Taylor dispersion method

Experimental purpose: Principal objective of the work

2. SELECT the Experimental Purpose from the list provided.

Comment (optional): Tracer response technique.

3. CLICK OK

OK

Cancel

SELECTION of # of Phases in Equilibrium and # of Constraints

Binary diffusion coefficient (* 10¹⁰ 1e-9 m²/s) as function of 2 variable(s)

Mixture: .alpha.-tocopherol + carbon dioxide

Phases in equilibrium:

1

Constraints:

1

Independent variables:

2

Phase of the Property Value(s)

SELECT the # of **Phases in equilibrium**. There is **1** phase; *fluid*.

SELECT the # of **Constraints**. There is **1** constraint in the present example; *the mole fraction of α -tocopherol = 0* to meet the infinite dilution requirement.

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)

Precision of the Property Value(s) * 10 1e-9 m2/s %

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



Multiple *samples* for a given component can be accommodated, but this is rarely needed.

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) Fluid (supercritical or subcritical phases) Units: Uncertainty: %

Independent variable 1 Fluid (supercritical or subcritical phases) %

Independent variable 2 Fluid (supercritical or subcritical phases) %

Definition of Measurement Results (Absolute vs. Relative) Direct value

NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

1) SELECT *Fluid* from the list provided for the **Phase of the Property Value**

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.

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) 10.7 * 10 1e-9 m2/s %

Constraint 1 (Fixed value of) Mole fraction of .alpha.-tocopherol of Fluid (supercritical or subcritical phases) Value: 0 Units: Dimensionless Uncertainty: %

Independent variable 1 Temperature of Fluid (supercritical or subcritical phases) Units: K Uncertainty: %

Independent variable 2 Pressure of Fluid (supercritical or subcritical phases) Units: MegaPa Uncertainty: %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experiment

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

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 variable

Phase of the Property Value(s) Fluid (supercritical or subcritical phases)

Constraint 1 (Fixed value of) Mole fraction of .alpha.-tocopherol Fluid (supercritical or subcritical phases)

Independent variable 1 Temperature of Fluid (supercritical or subcritical phases)

Independent variable 2 Pressure of Fluid (supercritical or subcritical phases)

Units: MegaPa Uncertainty: %

Definition of Measurement Results (Absolute vs Relative)
Direct value

Data presentation
Experimental values

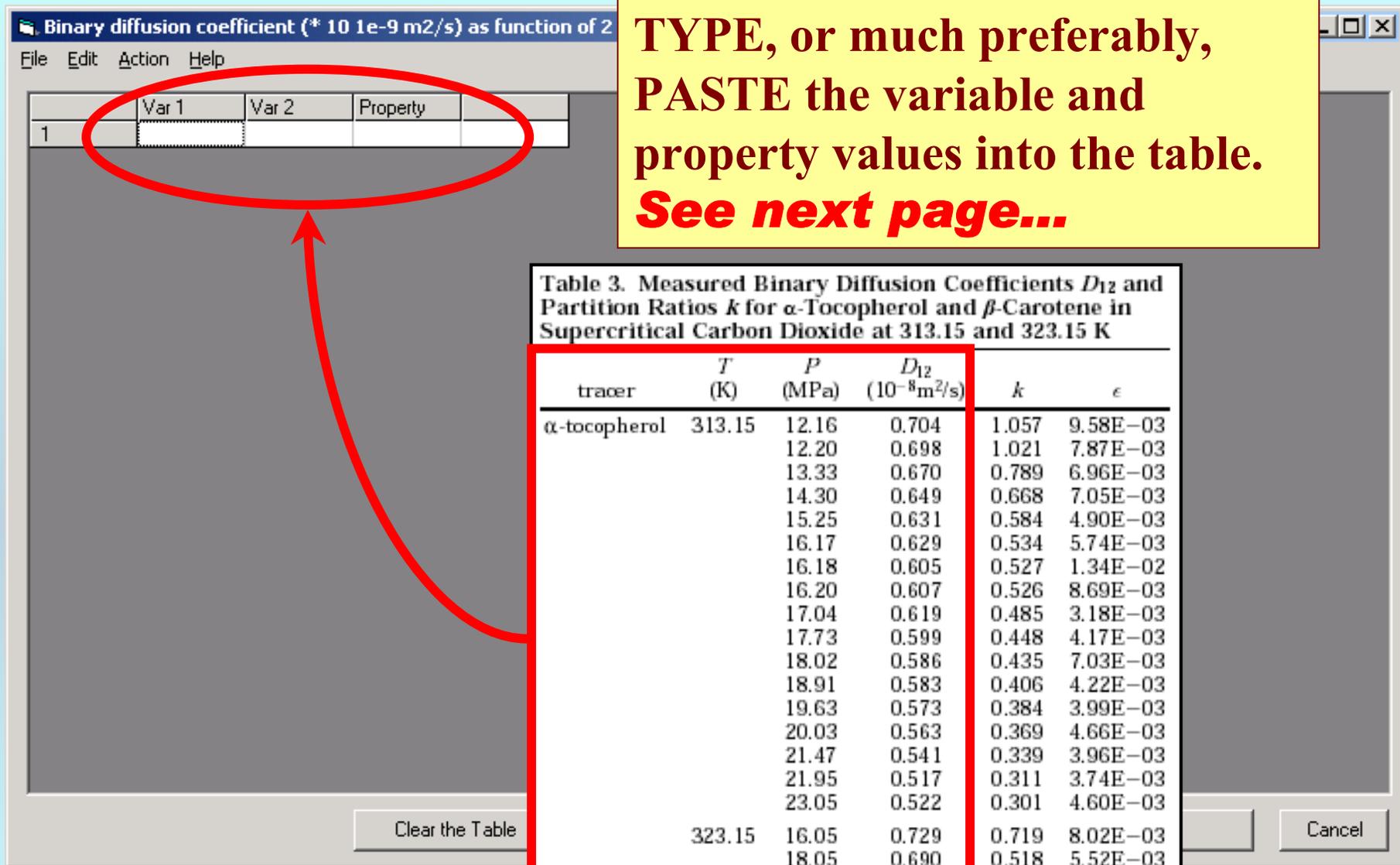
Comments (Optional): Tracer response technique.

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...

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} ($10^{-8} \text{m}^2/\text{s}$)	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		
β -carotene	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
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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
		21.95	0.517	0.311	3.74E-03
		23.05	0.522	0.301	4.60E-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

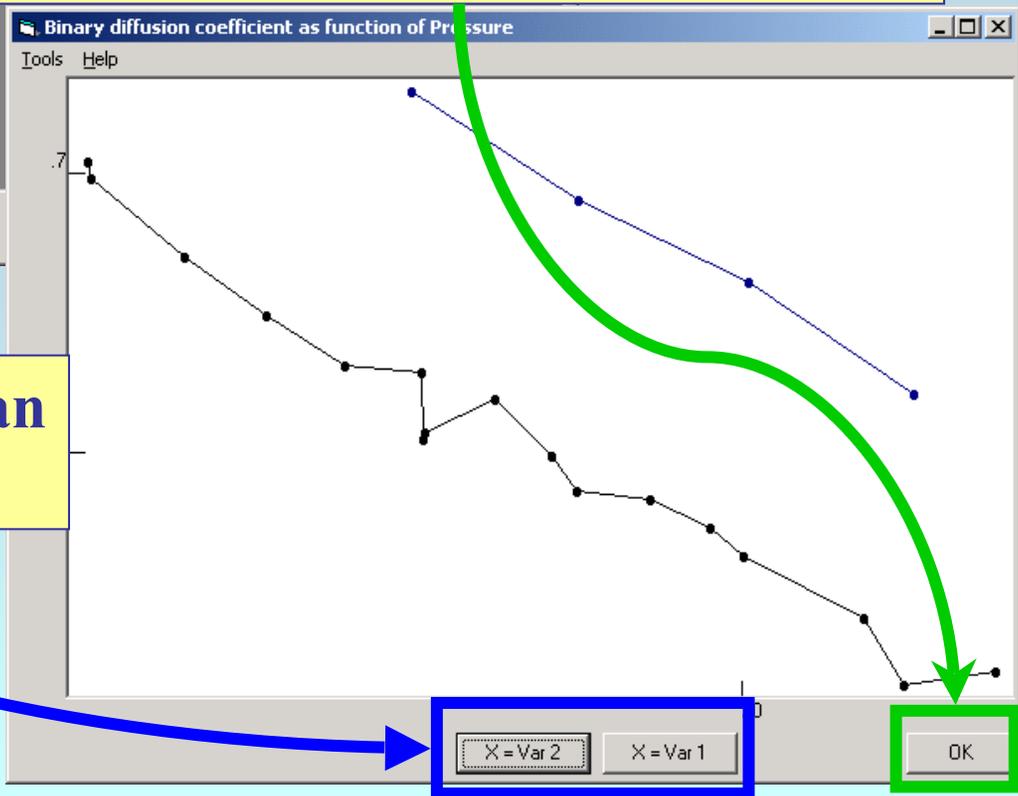
	Var 1	Var 2	Property
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15	313.15	21.47	0.541
16	313.15	21.95	0.517
17	313.15	23.05	0.522
18	323.15	16.05	0.729
19	323.15	18.05	0.690
20	323.15	20.08	0.661
21	323.15	22.07	0.621

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.

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
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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.