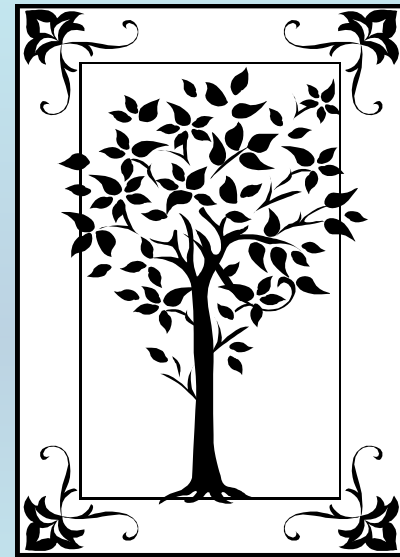


***GDC:***  
**ADVANCED OPERATION**

*For multiple data sets with near-identical metadata*

***Guided Data***  
***Capture (GDC)***



This tutorial describes  
**Advanced Operation**  
of the Guided Data Capture (GDC) software.

## **ADVANCED MODE**

This tutorial shows how to capture data for an *extended series of chemical systems (i.e, many compounds or mixtures)* for which the metadata (*i.e, method, uncertainties, constraints, and variables*) are the same (or nearly the same) for all of the data sets.

This approach is slightly more complex than the simpler *standard* GDC program operations, but eliminates much repetitive metadata capture.

## Guided Data Capture - Thermophysical and Thermochemical Data

File Edit **Tools** Help

Refer

**Configure**

und

Sample

Mixture

Reaction

Property

Data Tables

[-] 2003 zha & O

[-] carbon tetrachloride

... Sample 1 (cm;dc,fd;99m%,est)

[-] chloroform

... Sample 1 (cm;dc,fd;99m%,est)

[-] dichloromethane

... Sample 1 (cm;dc,fd;99m%,est)

... carbon tetrachloride + dichloromethane

... carbon tetrachloride + chloroform

... chloroform + dichloromethane

**CLICK on Configure in the Tools menu.**

**Guided Data Input: Configuration**

Configuration database: C:\Program Files\GDC\GDCLocal.mdb

GDC local database: C:\Program Files\GDC\GDC.mdb

Output folder: N:\TRC DataEntryFacility\8) Articles from JOURNALS\

Mode

Standard  Advanced

Accept Cancel

**1. SELECT**  
*Advanced.*

**2. CLICK**  
*Accept.*

**Guided Data Capture - Thermophysical and Thermochemical Data**

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

2003 zha & O

- carbon tetrachloride
  - Sample 1 (cm;dc,fd;99m%,est)
- chloroform
  - Sample 1 (cm;dc,fd;99m%,est)
- dichloromethane
  - Sample 1 (cm;dc,fd;99m%,est)
- carbon tetrachloride + dichloromethane
- carbon tetrachloride + chloroform
- chloroform + dichloromethane

**1. Capture all *bibliographic, compound identification, and sample* information.**

**2. Identify all *mixtures* after entering the *sample* information.**

**NOTE:** PDF help documents for capture of the above information are available on the Web ([www.trc.nist.gov](http://www.trc.nist.gov)), if needed.

The data-capture process for any property is *unchanged* in the **ADVANCED MODE** relative to the **STANDARD MODE** until *after* the last step; **Data Acceptance**.

**Data Acceptance** occurs on 2 forms; one for *single-valued* data and one for *tabular* data. Examples are given here.

Specific density at fixed conditions

Substance: methanol

Property set # 1 Phase 1: Liquid

Density at one  $T$  &  $p$

Independent variable: Temperature  
Value: 298.15 K Uncertainty:

Property value: 0.78732 g/cm<sup>3</sup> Precision: No of determinations:

Comment to this record:

Property and method Accept Cancel

CLICK Accept

Viscosity (mPa\*s) as function of 2 variable(s)

	Var 1	Var 2	Property
1	298.15	0.00	1.73
2	298.15	0.20	2.34
3	298.15	0.40	2.91
4	298.15	0.60	3.14
5	298.15	0.80	3.17
6	298.15	1.00	3.36
7	303.15	0.00	1.53
8	303.15	0.20	2.05
9	303.15	0.40	2.57
10	303.15	0.60	2.79
11	303.15	0.80	2.80
12	303.15	1.00	3.01
13	308.15	0.00	1.35
14	308.15	0.20	1.84
15	308.15	0.40	2.27
16	308.15	0.60	2.46
17	308.15	0.80	2.49
18	308.15	1.00	2.68
19	313.15	0.00	1.21
20	313.15	0.20	1.62
21	313.15	0.40	1.98
22	313.15	0.60	2.00
23	313.15	0.80	2.00
24	313.15	1.00	2.00
25	318.15	0.00	1.00

Viscosities =  $f(T,x)$

Clear the Table View plot Accept Cancel

CLICK Accept

Enthalpy of transition or fusion as single valued property

Substance: 1,3-dimethylbenzene

Property set # 1 Phase 1: Crystal Phase 2: Liquid Phase 3: Gas

Enthalpy of Fusion

Property value: 11.644 kJ/mol Precision: 0.012 No of determinations: 3

Comment to this record:

Property and method Accept Cancel

CLICK Accept

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

	Var 1	Property
1	276.94	0.0738
2	278.13	0.0725
3	279.95	0.0705
4	284.94	0.0542
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	308.18	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	376.69	0.0530

Composition =  $f(x)$

Clear the Table View plot Accept Cancel

CLICK Accept

In **ADVANCED MODE**: the screen will not change after **CLICKING *Accept***.  
*(see the next page for additional steps)*

In **STANDARD MODE**: the program returns to the *navigation tree* for entry of the next property, mixture, etc.

**TABULAR DATA:** Instead of returning to the main screen, you are returned to the screen for capture of **Constraint** and **Variable** information.

**SINGLE-VALUED DATA:** The screen does *NOT* change.

Specific density (g/cm<sup>3</sup>) as function of 1 variable(s)

Mixture: carbon tetrachloride + dichloromethane  
Phases: carbon tetrachloride + dichloromethane  
carbon tetrachloride + chloroform  
chloroform + dichloromethane  
Phase: New

Constraint 1 (Fixed value of): Temperature of Liquid Value: 303.15 Units: K Uncertainty: %

Constraint 2 (Fixed value of): Units: kPa Uncertainty: %

Units: Dimensionless Uncertainty: 0.0001 %

**1. SELECT the next MIXTURE or COMPOUND from the menu.**

Enthalpy of vaporization or sublimation at fixed conditions

Substance: benzene  
Property set: benzyl fluoride  
benzene  
toluene

Sample # 1

Independent variable: Temperature  
Value: 298.15 K Uncertainty: %

Property value

**2. Continue with data capture for the next MIXTURE or COMPOUND.**

**NOTE:** The **property identity**, **variables**, and **constraints** *DO NOT* need to be re-entered.



## **CAUTIONS:**

**1.** CLICK *Accept* only once after entry of each data set. Multiple CLICKS will add multiple (unwanted) data sets.

**2.** The **Value** fields do not clear after *Accept* is CLICKED. Be careful to change the **Property Value** for each data set, as needed.

See *Editing & Deletion Procedures* in the **HELP** menu on the *Main Screen*, if needed for removal or editing of incorrect entries.

**Enthalpy of vaporization or sublimation at fixed conditions**

Substance: benzene Sample # 1

Property set: benzyl fluoride  
benzene  
toluene

Independent variable: Temperature  
Value: 298.15 K Uncertainty:

Property value: 40.8 kJ/mol Precision: 2 No of determinations:

Comment to this record:

Property and method Accept Done

**CLICK *Done*, after CLICKING *Accept* for the final data set for the **Property**.**

**The program will then return to the *navigation tree* (i.e., the *Main Screen*) for continued data capture or program termination.**

**Specific density (g/cm3) as function of 1 variable(s)**

Mixture: carbon tetrachloride + dichloromethane

Phases: carbon tetrachloride + dichloromethane  
carbon tetrachloride + chloroform  
chloroform + dichloromethane

Phase New

Constraint 1 (Fixed value of) Temperature of Liquid Value: 303.15 Units: K Uncertainty:

Constraint 2 (Fixed value of) Pressure of Liquid Value: 101.3 Units: kPa Uncertainty:

Independent variable 1 Mole fraction of component 1 of Liquid Units: Dimensionless Uncertainty: 0.0001 %

Definition of Measurement Results (Absolute vs Relative) Direct value

Data presentation Experimental values

Comments (Optional):

Property and method Numerical Data Done

## Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference

Compound

Sample

- 2003 zha & O
  - carbon tetrachloride
    - Sample 1 (cm;dc,fd;99m%,est)
  - chloroform
    - Sample 1 (cm;dc,fd;99m%,est)
  - dichloromethane
    - Sample 1 (cm;dc,fd;99m%,est)

**NOTE:** All of the data sets entered will be listed under the appropriate *mixture* or *sample*.

Data sets for *mixtures* are shown here.

- carbon tetrachloride + dichloromethane
  - ^1: VDN (Set 1), B Method:VIBTUB dVDN=0.00005 dX1=0.0001
- carbon tetrachloride + chloroform
  - ^1: VDN (Set 1), B Method:VIBTUB dVDN=0.00005 dX1=0.0001
- chloroform + dichloromethane
  - ^1: VDN (Set 1), B Method:VIBTUB dVDN=0.00005 dX2=0.0001

**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.***