

# METADATA AND NUMERICAL DATA CAPTURE: Uncertainties (General Description)

## **G**uided **D**ata **C**apture (GDC)



This tutorial describes  
**DATA CAPTURE:**  
for **Uncertainties and Precisions**  
with the **Guided Data Capture (GDC)** software.

**NOTE: In GDC 3.0 all *uncertainty* and *precision* information is captured on one form, as shown below. The form appears after the property and metadata (phases, constraints, etc.) are specified.**

Uncertainty information

Help

**Constraint: Temperature (K)**  
 Uncertainty ← *Most important*  
 Device specification  
 Repeatability

**Variable 1: Mole fraction of heptane (Dimensionless)**  
 Uncertainty ← *Most important*  
 Device specification  
 Repeatability

**Property: Vapor or Sublimation pressure (kPa)**  
 Combined uncertainty ← *Most important*  
   
 Device specification  
 Repeatability  
 Curve deviation

OK Cancel

The **constraints**, **variables**, and **property** shown will correspond to the particular data being captured.

**NOTE: Entry of uncertainty information is highly recommended, but *OPTIONAL*.**

The most important quantities are the Uncertainty (for the **property**, **constraints** and **variables**) and Combined Uncertainty (for the **property** only).

The other quantities are measures of **precision** only and represent **lower limits** for the uncertainties.

Definitions follow...

**Constraint: Temperature (K)**

- Uncertainty  *Most important*
- Device specification
- Repeatability

**3 measures of uncertainty/precision are shown for each constraint, variable, and property.**

**The property has two additional quantities described later.**

**You can select to enter any or all of these. Additional fields associated with the quantity appear after selection. (Select by checking the *check box*)**

**The following pages show each uncertainty/precision type.**

**Variable 1: Mole fraction of heptane (Dimensionless)**

**Uncertainty**

Device specification

Repeatability

Value:   %

Level of confidence:  %

Uncertainty is the most important quantity for **variables** and **constraints**. This quantity is the *Expanded Uncertainty* described in *J. Chem. Eng. Data*, 2003, 48, 1344.

It includes the uncertainty arising from all sources, but *does not include propagation of uncertainty from other constraints or variables*.

The **Value** for the *entire data set* can be entered as an *absolute value* or *percentage*. (Select the % check box for percentages)

The **Level of confidence** is assumed to be 95%, but you can change this value, if necessary.

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**NOTE:** If necessary, *Uncertainties* associated with *individual data points* can be entered in the *Data Table Form* which follows the *Uncertainty Info Form* in the GDC software.

Variable 1: Mole fraction of heptane (Dimensionless)

Uncertainty

Device specification Value:   % Level of confidence:  % Evaluator:

Repeatability

Device Specification is a type of **precision**.

*Device specification* allows reporting of *device calibration information*. This does not include uncertainties associated with use of the device in the experimental apparatus.

For example, a thermometer could have a *Device Specification* value of 0.01 K (based on calibration), but the uncertainty in the temperature measurements might be much larger.

The *Device Specification* value is one measure of the **lower limit** for the uncertainty.

The **Level of confidence** is assumed to be 95%, but you can change this value, if necessary.

Variable 1: Mole fraction of methyl tert-butyl ether (Dimensionless)

Uncertainty

Device specification

Repeatability      Value:   %      Standard Deviation of a Single Measurement       Repetitions:

Repeatability is another type of **precision**.

*Repeatability* is defined as:

Closeness of the agreement between the results of successive measurements of the same measurand carried out under the **same** conditions of measurement.

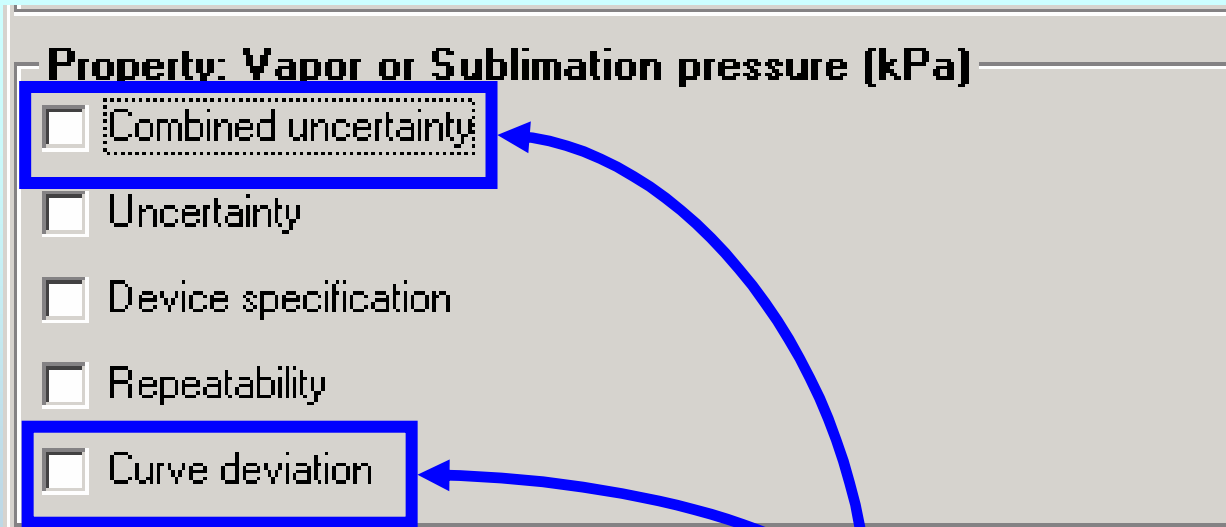
Repeatability is expressed in GDC as: the *Standard Deviation of a Single Measurement* or the *Standard Deviation of the Mean*. (Mathematical formulations are given in the HELP file for the Uncertainty Information form.)

The *Repeatability* value is another measure of the **lower limit** for the uncertainty.

The **Level of confidence** is assumed to be 95%, but you can change this value, if necessary.

**Property: Vapor or Sublimation pressure (kPa)**

- Combined uncertainty
- Uncertainty
- Device specification
- Repeatability
- Curve deviation



The PROPERTY has 2 additional representations:

- 1) Combined Uncertainty: This is like the *Uncertainty*, but it includes *uncertainty propagated* from the variables and constraints. This is the most important representation of uncertainty.
- 2) Curve deviation: This is another measure of the *lower limit* for the uncertainty

Property: Vapor or Sublimation pressure (kPa)

Combined uncertainty    Value:   %    Level of confidence:  %

Uncertainty

Device specification

Repeatability

Curve deviation

The method of determination is selected here.

- **Combined Uncertainty** is the most important quantity for properties. This is the *Combined Expanded Uncertainty* described in *J. Chem. Eng. Data*, 2003, 48, 1344.
- This quantity includes the uncertainty arising from all sources, and includes propagation of uncertainty from the constraints or variables.
- The quantity can be entered as an *absolute value* or *percentage*. If necessary, *Combined Uncertainties* associated with individual data points can be entered in the *Data Table Form* which follows the *Uncertainty Info Form*. (Leave the *Value* field blank, if the uncertainties will be entered directly in the *Data Table Form*.)
- You should select how the values were determined from the indicated pull-down menu. (shown in the **red** box above)
- The **Level of confidence** is assumed to be 95%, but you can change this value, if necessary.

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**NOTE:** If necessary, *Uncertainties* associated with *individual data points* can be entered in the *Data Table Form* which follows the *Uncertainty Info Form* in the GDC software.



Property: Vapor or Sublimation pressure (kPa)

Combined uncertainty

Uncertainty

Device specification

Repeatability

Curve deviation

RMS:   %

Equation type:

The equation type or name can be entered here as text.

Curve deviation is another type of **precision**.

*Curve deviation* is defined as:

The root-mean-square deviation from a specified curve.

The *Curve deviation* value is another measure of the **lower limit** for the uncertainty.

The value can be expressed as an absolute value or percentage.

The **Level of confidence** is assumed to be 95%, but you can change this value, if necessary.

**Uncertainty information** [X]

Help

**Constraint: Pressure (kPa)**

Uncertainty Value:   % Level of confidence:  %

Device specification

Repeatability

**Variable 1: Temperature (K)**

Uncertainty Value:   % Level of confidence:  %

Device specification

Repeatability

**Variable 2: Mole fraction of diethyl carbonate (Dimensionless)**

Uncertainty Value:   % Level of confidence:  %

Device specification

Repeatability Value:   %  Repetitions:

**Property: Viscosity (\* 0.001 Pa\*s)**

Combined uncertainty Value:   % Level of confidence:  %

Uncertainty

Device specification

Repeatability

Curve deviation

**Click *OK*, when the form is complete.**

All definitions are based on the following documents:

Definitions and descriptions of all quantities related to the expression of uncertainty in GDC conform to the;

*Guide to the Expression of Uncertainty in Measurement, ISO (International Organization for Standardization), October, 1993.*

These ISO recommendations were adopted with minor editorial changes as the;

*U.S. Guide to the Expression of Uncertainty in Measurement. (commonly referred to by its abbreviation; the GUM).*

The recommendations have been summarized in;

*Guidelines for the Evaluation and Expression of Uncertainty in NIST Measurement Results*

This final document is available via free download from the Internet

*(<http://physics.nist.gov/cuu/>).*

**A more complete discussion of the uncertainty terms used here is given in *J. Chem. Eng. Data*, 2003, 48, 1344-1359.**

*Note: This article provides much more detail than is necessary for use of GDC.*

# END

**Continue with data capture...**