

Measurement Uncertainty Service Tool

«MUST» of IFA

User manual



**Institute for Occupational Safety and Health
of the German Social Accident Insurance**

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Index of abbreviations

Abbreviation	Full name
AK	(preliminary) acceptable cancer risk
AS	assessment standard
ERR	exposure risk relationship
I-dust	inhalable dust
IFA	Institute for Occupational Safety and Health
ILV	International Limit Value
k	coverage factor
L	litres
m ³	cubic meters
µg	micrograms
mg	milligrams
min	minutes
mL	millilitres
MU	measurement uncertainty
OEL	occupational exposure limit
PDS	Process Datasheet
R-dust	respirable dust
TK	tolerable cancer risk
U	expanded measurement uncertainty

Table 1: Index of abbreviations

Introduction

A measurement procedure for determining hazardous substances at workplaces essentially comprises two stages: sampling and analysis. The measured value depends on both stages. The true value is never known and, therefore, always subject to uncertainty. The measured value is only an estimate that is influenced by various factors. Measurement uncertainty (MU) is a parameter related to the result of a measurement and which characterises the scatter attributable to a measured value.

The purpose of assessing measurement uncertainty is to provide accurate information about influences X_i on a quantity $Y = f(X_i)$ that needs to be determined. For each influence X_i two values are determined from the available information: the sensitivity coefficient c_i and the standard deviation σ_i . The combination of coefficients and standard deviations for each influence produces the combined standard deviation $\sigma_c = \sqrt{\sum_i c_i^2 \cdot \sigma_i^2}$.

Assuming that the scatter of the measured values due to influences X_i corresponds at least approximately to a normal distribution, we use this to calculate the so-called extended measurement uncertainty: $U = k \cdot \sigma_c$, where U specifies the extended measurement uncertainty and k the coverage factor. If one assigns a probability of 95 % to the range $y \pm U$, the coverage factor is $k = 1,96$.

To calculate the measurement uncertainty (MU), we start by collecting all influences X_i . We then record the deviations for these influences, which we can obtain from the manufacturer's specifications, from test certificates, standards or via process validation.

Not all stages in process validation have an influence on the measurement uncertainty. It is important to cover the following influences:

- Sampling,
- If applicable, transportation of samples to the laboratory (only particulate/vapour mixtures),
- Sample preparation,
- Calibration of the measuring device(s),
- Recovery of the substance,
- Precision of measurement results under repeatability or reproducibility conditions,
- Drift of measuring devices,
- Influence of temperature (for all procedures except metals/metalloids, for gases and vapours, if the sample carrier has an influence),
- Influence of humidity (for all procedures except metals/metalloids)

First, we create a list of influences and their deviations. As mentioned above, each of these influences is subject to uncertainty. These uncertainties can be divided into systematic and random deviations. Such a list forms the basis of any assessment of measurement uncertainties.

The Guide to the Expression of Uncertainty in Measurement (GUM) interprets standard uncertainties as standard deviations σ , and this application follows the interpretation of the GUM. As the true values of the s will always remain unknown, we calculate their estimated values. This manual provides the calculation of estimates for such standard deviations. To calculate the sensitivity coefficients, we set up the mathematical model for the desired quantity Y and then then pick its first derivative with respect to the X_i . Sensitivity coefficients weight the influence of an uncertainty component on a (measurement) parameter. In addition, they account for the correct units of the combined standard deviation.

In future, this application should be able to calculate the extended measurement uncertainty for most IFA-validated methods that determine airborne chemical substances at workplaces. The application, called Measurement Uncertainty Service Tool (MUST for short), comprises mathematical models for three procedures: Thermodesorption, Extraction and Metals with ICP-MS. It also records all influences on the measured value with their respective deviations in a Model Datasheet. In addition, one has to import data from process validation.

To use this application within the IFA, there is a so-called Process Datasheet (PDS) for entering any identified process parameters, such as recovery and calibration. To use the app outside IFA, separate datasheets have been drawn up, which are reserved exclusively for entering data with relevance to measurement uncertainty. These datasheets are automatically downloaded together with the application and are named according to the procedures to which they belong:

- Thermodesorption_Calibration&Recovery,
- Extraction_Calibration&Recovery,
- Metals_Calibration&Recovery.

MUST imports both the Model Datasheet and the relevant parameters of the associated procedure/process (validation data) from the Process Datasheet (PDS) or the above-mentioned files. They are then directly included when calculating the extended measurement uncertainty, and individual parameters can be edited where necessary. In addition, to obtain the extended measurement uncertainty, MUST calculates the measurement value β taking into account systematic effects.

A list is returned for these results, indicating the uncertainty share of the individual parameters in the extended measurement uncertainty and which parameters thus have the greatest influence on the measured value. One can save the results to a separate Excel file.

Please note:

Compatibility of IFA Process Datasheets

Gases/vapours: version 11 or higher

Metals: version 3 or higher

Important! The app CANNOT import older process datasheets.

The recovery and calibration data files from the downloaded file folder («Thermodesorption_Calibration&Recovery», «Extraction_Calibration&Recovery» and «Metals_Calibration&Recovery») are independent of the version and can be used instead of the PDS.

1 Brief overview: How to Use the App

The user interface of MUST consists of several parts, referred to as «tabs» in this document. Under each tab, there are several areas that are separated from each other by boxes. These areas are called «sections» here.

This chapter provides an initial overview of how to import information on measurement procedures into the app, enter measurement data and export the finished result from the app. More detailed explanations of the individual tabs, sections and boxes can be found in the relevant sections in Chapter 2.

1.1 Fundamentals

We start by filling in the «Basic Information» tab. Go to the «Fundamentals» section and enter general information, e. g. the person carrying out the work, loading techniques, assessment standards or the validation date (see boxes 1 - 6 in Figure 1) These details are not required for the calculation, but they are important for documentation purposes, as they are also saved to the output file.

Field Number	Field Name	Value / Selection
1	Executing Unit	IFA, Section 2.0
2	Operator	
3	OELV	ILV
4	Validation date	
5	Application	Aerosolgenerator
6	Standard Operating Procedure	

Figure 1: Section «Basic Information» in tab «Fundamentals»

1.2 Information on the procedure

Under the «Basic Information» tab, one chooses the method/process/procedure, provides the name of the analyte and the assessment standard (in the «Information on the procedure» section, see boxes 7 - 9 in Figure 2).

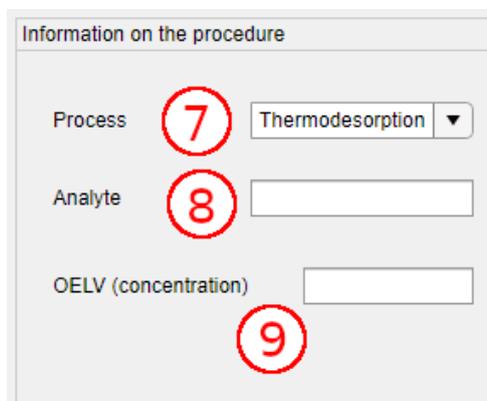


Figure 2: Section «Information on the procedure» in tab «Fundamentals»

1.2.1 Available measurement methods/procedures

Method 1 - Thermodesorption

For thermodesorption procedures, we need to specify whether the Process Datasheet or the datasheets in the download folder contain recovery data on the temperature and humidity that can be imported by the app. In section 2.1.3, «Particle-Vapours / Gases-Vapours / Thermodesorption», one must tick the relevant checkboxes (see box 10 in Figure 3). If these boxes have been ticked, but there is no data, the app returns an error message (more on error messages in Chapter 3, «Instructions for Handling Error Messages»). No further details are required for this method in the «Fundamentals» tab.

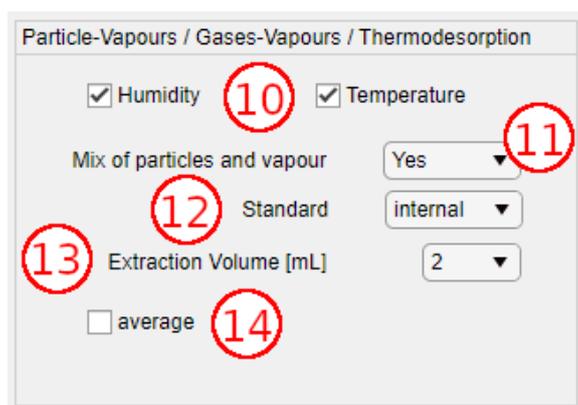


Figure 3: Section «Particle-Vapours / Gases-Vapours / Thermodesorption» in tab «Fundamentals»

Method 2 - Extraction

As in method 1 (Thermodesorption), we need to specify whether the Process Datasheet or the datasheets from the website contain recovery data on the temperature and humidity that can be imported by the app (see also section 2.1.3, «Particle-Vapours / Gases-Vapours / Thermodesorption»). One must tick the relevant checkboxes (see box **10** in Figure 3)), check the boxes **11 - 14** in this section (see Figure 3) and change if necessary. The boxes indicate whether the procedure in question analyses a particulate-vapour mixture, whether an internal standard is used or not. In addition, they indicate the extraction volume and whether the measured values are mean values from several analyses. Further details on each of the menus can be found in section 2.1.3.

Method 3 - Metals ICP-MS

The section «Particle-Vapours / Gases-Vapours / Thermodesorption» (see section 2.1.3 in this manual) is not applicable to the «Metals ICP-MS» procedure and has therefore been disabled. Note the «Metals ICP-MS» section (see section 2.1.4 in this manual) on this point. One must specify the fraction to which the assessment standard refers, as well as the digestion type and the dilution factor (see boxes **15 - 17** in Figure 4). Further details on each of the boxes can be found in section 2.1.4, «Metals ICP-MS».

The image shows a software interface window titled "Metals_ICP-MS". It contains three rows of configuration options, each with a red circle containing a number: 15, 16, and 17. Row 1: "Fraction associated to OELV" with a dropdown menu showing "R". Row 2: "Digestion" with a dropdown menu showing "Open". Row 3: "Dilution" with a dropdown menu showing "10".

Figure 4: Section «Metals ICP-MS» in tab «Fundamentals»

1.3 Input-Calculate-Save

After entering and checking the information under the first tab, go to the second tab, «Import-Calculate-Save». We now need to provide details regarding the influencing factors in two separate files: in the Model Datasheet and either in the Process Datasheet for use within IFA or in the datasheets obtained from the download folder

(i.e. («Thermodesorption_Calibration&Recovery», «Extraction_Calibration&Recovery» and «Metals_Calibration&Recovery») for use outside IFA.

The Model Datasheet contains general information on the selected procedures. The Process Datasheet or the datasheets from the download folder contain the calibration and recovery data of the analyte from the validation tests. Make sure that all the necessary data from the validation of the procedure have been saved to the PDS or the associated datasheet and – in the case of internal IFA calculations – that the PDS is compatible with the app (gases/vapours from version 11, metals from version 3).

We recommend uploading these two files first. To do so, click «Import» (see box 18 in Figure 5).

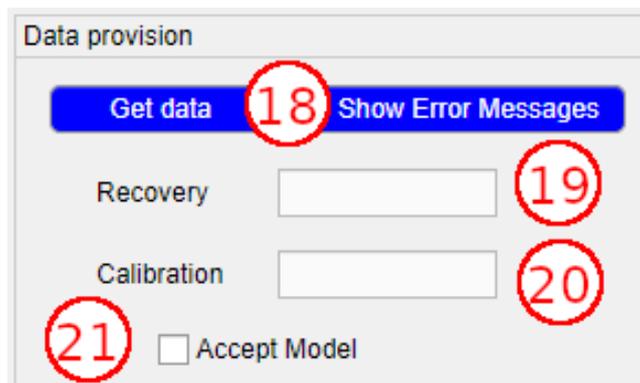


Figure 5: Section «Data provision» in tab «Input-Calculate-Save»

1.4 Data Provision

After a short wait, a new folder window opens in the Explorer, «Select File to Open», prompting us to select either the PDS or the datasheet for the procedure for which we want to calculate the measurement uncertainty. Click «Open» to confirm, whereupon both files (Model Datasheet and PDS/datasheet) are uploaded simultaneously. As the Model Datasheet contains general details and often does not need editing, it is located in the top folder of the download archive and is loaded automatically. When the two datasheets are opened, the app checks the data that are imported (this may take some time). If there are complications during import, error messages are presented in a separate window. For a description of potential errors and recommended remedies, see Chapter 4. We can also retrieve error messages later with a click on «Show Error Messages» (see box **18** in Figure 5).

1.5 Checking Imported Data

If the import is successful, the app provides the recovery, calibration and model data under the relevant tabs. Next, we need to check the following:

- Have all data («Recovery», «Calibration», «Model») been imported?
- Do the target concentrations in the app match those in the Process Datasheet?
- Is the number of data items [N] under the «Recovery» tab correct?
- Is the number of calibration points under the «Calibration» tab correct?
- Does the «Model» tab contain the relevant model parameters for the procedure?

Depending on the procedure, it is possible to edit the specifications for the device drift and the sampling head under the «Model» tab. For further details on the Model Datasheet and possible changes to the model parameters in the app, see section 2.5, «Model».

Please note: To confirm that the entries under the «Model» tab have been checked, we must place a tick in the «Model OK» checkbox under the «Import-Calculate-Save» tab (see box **21** in Figure 5). Unless we provide this confirmation, the app cannot calculate the MU and will return an error message.

1.6 Calculating Measurement Uncertainty

As the app now has all the required details for the procedure, we can now enter the measured values (section: «Validated Concentration»).

First, we need to specify the mass or concentration of the analyte (either box **22** or boxes **22a - 22b**). We also need to enter the volume flow (box **24**), the sampling duration (box **25**) and – for the «Metals ICP-MS» procedure – the digestion volume (box **26**, see Figure 6).

Figure 6: Details of measured values for «Metals ICP-MS», on the left and for «Extraction» on the right, if the determination of a mean value is required.

Based on the procedure at hand, the app now has all the information it needs to calculate the measurement uncertainty for a measured value. To trigger the calculation, click «Calculate» (box **27**, see Figure 7).



Figure 7: Buttons under the «Import-Calculate-Save»-tab

Next, the system displays the adjusted measured value β (box **29**), the combined standard uncertainty u_c (box **30**) and the extended measurement uncertainty U (boxes **30 - 31**, see Figure 8) in the «Result» section.

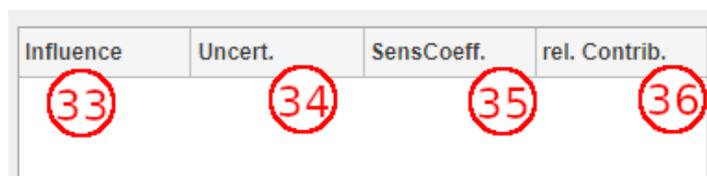
Result	
29 beta [mg/m ³]	<input type="text" value="0.00e+00"/>
30 u_c	<input type="text" value="0.00e+00"/>
31 U [mg/m ³]	<input type="text" value="0.00e+00"/>
32 U [%]	<input type="text" value="0"/>

Figure 8: Berechnung von U

The minimum requirements for measurement procedures according to DIN EN 482, ISO 20581 or TRGS 402 are referring to U [%] (extended measurement uncertainty in per cent of β , box **32**, see Figure 8).

1.7 Percentages of Uncertainty Parameters

In the right-hand table next to the calculation, the relevant influencing factors (box **33**, see Figure 9) are indicated together with their relative percentage of the total extended measurement uncertainty (box **36**, see Figure 9). Further details about this table and each box and button can be found in section 2.2.



Influence	Uncert.	SensCoeff.	rel. Contrib.
33	34	35	36

Figure 9: Table of influencing factors

As a final step, one may save the calculation and its results. For every single concentration (or mass) of each substance for which the measurement uncertainty is calculated, one needs to save the results to a separate file. Data are exported in the xlsx format (i. e. MS Excel).

To trigger this, click «Save» (box **28**, see Figure 7). Again, a new Explorer window is presented, «Select File to Write», prompting us to select a suitable file location. In addition to the results of the calculation, the app also saves to the Excel file all the data that has been imported or entered into the app, as well as any error messages, the relevant model data and the sensitivity coefficients.

Please note: This Excel file should not be overwritten but must always be saved separately. Overwriting it would lead to errors in the Excel worksheets.

2 Layout and Structure of the App

After the brief overview in Chapter 1, outlining the functions of MUST, we will now provide more detailed explanations of each box, the underlying functions and calculations. Like Chapter 1, the structure of Chapter 2 is based on the tabs and sections of the application.

2.1 Fundamentals

This tab is the starting point. It is for specifying general details of the procedure for which we want to obtain the MU. To display help and information on a given box, simply move the cursor over it (mouse over fields).

2.1.1 Basic information

All the boxes in this section (see Figure 1) are provided for documentation purposes. However, they do not influence the calculation. They may be saved by the app together with the other information on the measurement uncertainty calculation (by clicking «Save», box **26**, see Figure 7).

Box 1 - Name of the laboratory. This is where one can choose a laboratory of the Chemical and Biological Hazards department of the IFA. It is also possible to add the own laboratroy: simply choose «Free Text» on the menu and make an entry

Box 2 - Person calculating the MU. Potential queries should be directed this person directly. Ideally, this should be the same person who validated the method.

Box 3 - Specify here the assessment standard to which the validation of the relevant substance relates or the assessment standard under which the substance is being assessed. The following choice is presented: Occupational Exposure Limit (OEL) – Exposure Risk Relationship and Acceptance Concentration (ERR, AC) – Exposure Risk Relationship and Tolerance Concentration (ERR, TC) – both: ERR, AC and TC – International Limit Values (ILVs) This box, too, allows us to enter further assessment standards manually, as free text.

Box 4 - This free text box, «Validation from», is for entering the year of validation.

Box 5 - To ensure full documentation of the measurement procedure, we also need to specify the application technique. The following options are provided in the dropdown menu: «Aerosolgenerator», «Spiking/Loading of sampling material», «Suspension», «Dynamic test gas stream», «Gasmouse», «Dynamic test gas stream and gasmouse», «Spiking/Loading and test gas stream», as well as a «free text» box where we can enter other techniques.

Box **6** - Specify here the relevant standard operating procedures (work instructions), e. g. the numbers of the relevant IFA folders or references to process specifications such as those provided by the German Research Foundation (DFG) or those within the IFA's Q.wiki or the measurement system risk assessment of the German social accident insurance institutions (MGU).

2.1.2 Information on the procedure

Boxes **8** and **9** in this section are necessary for documentation purposes, without affecting the calculation. They are saved by the app together with the other information on the measurement uncertainty calculation (see «Save» button, box **26**, in Figure 7).

Box **7** - One specifies here the procedure for which one wants to calculate the measurement uncertainty. The available calculation models at this point are currently «Thermodesorption», «Metals ICP-MS» and «Extraction». This choice is the basis for the calculation. If we select a different procedure, the system automatically deletes all previously entered specifications (imported files and measured values). This selection decides which worksheet is to be imported from the Model Datasheet and which structure the app should expect in the Process Datasheet.

Box **8** - This is a free text box where we can specify the substance for which we want the app to calculate the measurement uncertainty or the substance that has been validated.

Box **9** - This is a free text box where we may enter the limit value (and unit) of the assessment standard. These details will be exported to the result file.

2.1.3 Particle-Vapours / Gases-Vapours / Thermodesorption

This section is only active if «Thermodesorption» or «Extraction» has been selected in box **7**. All the details here affect what the app imports. If we have selected «Thermodesorption», boxes **10** - **14** are disabled.

Case 1: «Thermodesorption»Method

If we have selected «Thermodesorption» as a procedure under «Process Details», then the two checkboxes for humidity and temperature are visible and selected (see box **10**, Figure 3). If no data has been specified for the procedure that is to be validated and if no data has been placed in the underlying PDS, it is important to untick the relevant box. Otherwise the software will return an error message upon clicking «Calculate» under the «Import-Calculate-Save» tab. The app will still calculate the measurement uncertainty, but the error message should alert us to the fact that these influences are not specified in the validation, even though the standard demands that they should be there. The same happens if either

the temperature or the humidity in the tests is outside the range specified in the standard. If «Humidity» and «Temperature» continue to be selected, the relevant data from the PDS «Gases Vapours» are placed under the «Recovery» tab upon import and are included in the calculation of the extended MU. All other boxes (i. e. **11 - 14**, see Figure 3) remain disabled.

The app will abort its calculations if wrong units of measurement have been specified in the Process Datasheet. For «Thermodesorption», the measured value must be provided in $[ng]$ or $[mg]$. Also, recovery data must contain at least three target concentrations and at least six repeat concentrations for each target concentration. The app will abort its calculations, if it cannot find such data.

Case 2: «Metals ICP-MS»method

For this procedure, all boxes in the «Particle-Vapours / Gases-Vapours / Thermodesorption» section remain disabled.

Case 3: «Extraction»method

A range of further process parameters are requested in addition to the two checkboxes «Humidity» and «Temperature». A dropdown menu entitled «Mix of particles and vapour» (see box **11** in Figure 3) is presented, prompting us to specify whether the substances under assessment are particulate-vapour mixtures (click «Yes» in the menu) or gases/vapours (click «No» in the menu). For particulate-vapour mixtures, the app will take into account the sampler as an influencing factor.

The second dropdown menu (see box **12** in Figure 3) allows us to specify whether an internal standard is used («internal») or not («external»).

In the last menu we need to select the extraction volume (see box **13**). Random and systematic deviations of the volumetric measuring devices are saved according to the extraction volume for calculating the measurement uncertainty. We can choose between the following extraction volumes: 2 mL, 2.5 mL, 3 mL, 4 mL, 5 mL and 10 mL. The uncertainty components of the extraction volumes refer to the worst-case values of the random and systematic errors of the volumetric measuring devices that are used. Other volumetric measuring devices for different extraction volumes are not currently accounted for but can be added on request.

Box 14: If this box is ticked, the resulting value is a mean value arising from two measurements. Two measured values are therefore required (see Figure 6). The app will assume that they have been obtained in the same manner (same sample and sampling time, same volume flow and same extraction solution). If we use a separate column for the second value (first column polar, second non-polar), then we need to enter a second set of calibration values in the Process Datasheet, whereupon the app will automatically assume that these calibration values apply to the second measured value.

2.1.4 Metals ICP-MS

If we specified «Metals ICP-MS» in the «Information on the procedure» section, then the boxes in this section will influence the calculations. In all other instances, they will remain disabled.

Box **15** - This dropdown menu requires us to select a dust fraction for the assessment standard (AS). In some cases, there are different assessment standards for metals/met-alloids in the respirable dust fraction and in the inhalable dust fraction. If this is the case, one must make sure the value in box **9** matches the fraction specified in box **15**. The app refers for the calculation to the dropdown menu in the «Metals ICP-MS» section, box **15**, and takes the uncertainty of the sampler from the Model Datasheet for the fraction selected here.

Box **16** - Specify here digestion type for which one wants to import data from the PDS. one can choose between «Open» and «Microwave-Assisted».

Box **17** - This is where one sets the dilution. We can choose between 10 (for 1:10), 100 (for 1:100) and 1,000 (for 1:1,000). No other dilution factors are currently available but can be added on request.

2.2 Data Provision / Input-Calculate-Save

This tab is both for importing data and for calculating the extended measurement uncertainty U . The «Data Provision» section contains two buttons (box **18**), two comment boxes (**19** and **20**) and a checkbox (**21**).

Box **18** - To import data, click «Get Data» (see Figure 5). Next, an explorer window is opened («Select File to Open»), prompting the selection of the Process Datasheet for the chemical substance that has been validated. As soon as the selected file is confirmed, the data is imported into the app. At the same time, the Model Datasheet is also imported (the file is located in the same folder as the app and therefore does not need to be selected separately). More details about the Model Datasheet can be found in Chapter 3.

During the import, the app verifies the data from the PDS. If the recovery or calibration data has been imported incorrectly, an error message is presented in boxes **19** and **20** (see Figure 5). However, in addition to these error messages which merely refer to the import of recovery and calibration data, there will also be further error messages about the actual data itself. Error messages do not necessarily mean that a calculation of the MU cannot be carried out but may also provide information for the interpretation of the MU result or indicate errors in the calculation, import or handling of data which may have an impact on the result but may not necessarily be critical.

The data is imported and the app calculates the calibration curve from the calibration data, before we need to click «Calculate» to start all other calculations (box **27**). This is necessary in order to calculate the underlying measured value of the analysis device (counting rate, area units, etc.) on the basis of the results of the analysis device (mass and concentration). This underlying measured value is then presented in box(es) **23** (see Figure 6). As the calibration curve was already calculated during import, only a note (error message) is presented at this stage if the calibration curve is calculated with weighted regression. If analysis devices only calculate the regression of calibration under the method of least squared errors, they may overlook the fact that in most cases the variance of calibration values increases with a rise in concentration/mass. If there is an infinite number of calibration concentrations, both methods lead to the same regression parameters. However, the variance is only properly detected in a weighted calculation. Therefore, the app needs to calculate with the weighted regression if the variance is not constant. One consequence is the back-calculated value that appears in box(es) **23** which may not match those of the analysis device if the analysis device performs calculations using a simple linear regression.

The meaning of the individual messages and corresponding instructions are described in more detail in Chapter 4. Critical errors are reported directly in a pop-up window during import. Error messages that have no influence on the calculation of the MU are reported in box **19** or **20** but are only visible when we click «Show Error Message» (box **18**, see Figure 5). **Box 21** - This checkbox must always be ticked before the MU is calculated. Before doing so, the data must be checked under the «Model» tab. Further details about the «Model» tab can be found in section 2.5. The box for the model can be ticked after all entries

in the Model Datasheet have been checked for plausibility, especially whether the editable influencing factors «Sampler» and «Device Drift» have been selected correctly.

2.2.1 Validated Concentration

In this section the key data for the validated concentration or mass needs to be entered. As a decimal separator a full stop (period) is used instead of a comma. The app generally calculates the measurement uncertainty for one specific measured value at a time. If, however, the MU of a procedure needs to be obtained, it has to be calculated for at least three concentrations of the minimum measuring range. Enter the concentrations separately in the app and save them as separate files. A simultaneous calculation is not possible. The Process Datasheet does not need to be imported each time. It is sufficient to edit either box **22** or boxes **22a** and **22b** and then to click **27**, «Calculate».

Table 2 describes the concentrations depending on the assessment standards for which the MU needs to be calculated.

Assessment Standard	Minimum Measuring Range	Concentrations for MU
OEL	0.1 - 2 OEL	0.1; 1 (or 0.5); 2 OEL
AC under ERR	0,2 - 2 AC	0,2; 1 AC; 2 AC
TC under ERR	AC - 2 TC	1 AC; 1 TC; 2 TC
AC and TC	0.2 AC - 2 TC	0.2 AC; 1 AC; 2 TC

Table 2: Relationship between minimum measuring range of the method and the MU being calculated for the whole process

Case 1: Thermodesorption

If the «Thermodesorption» method in the «Information on the procedure» section in the «Fundamentals» tab is selected, the analyte is returned in nanograms [*ng*] in box **22** (see Figure 6).

It is recommended to compare the measured value in the greyed-out box **23** with the value for the analysis device. If the two figures do not match, it is possible that the analysis device has failed to take into account the increase in calibration variances (see discussion of the «Calculate» button, section 2.2). In box **24**, the standard volume flow of the procedure is given in litres per minute [*L/min*] and in box **25**, the standard sampling time of the procedure is given in minutes [*min*]. Box **26** remains disabled and is irrelevant for the «Thermodesorption» method. It is important to use a full stop (period) «.» as a decimal separator, not a comma.

Case 2: Metals ICP-MS

If the ICP-MS procedure has been selected in the «Fundamentals» tab in the «Information on the procedure» section (see Figure 2), box **22** (see Figure 6) will show the concentration in micrograms per litre [$\mu\text{g/L}$]. Box **23** remains disabled. The signal intensity that is specified here in counts per second [cps] can be compared with the value shown for the analytical device. If the two figures do not match, it is possible that the analytical device has failed to take into account the increase in calibration variances (see discussion of the «Calculate» button, section 2.2). In box **24**, the standard volume flow of the procedure is given in litres per minute [L/min] and in box **25**, the standard sampling time of the procedure is given in minutes [min]. The standard digestion volume is specified in millilitres [mL] in box **26**. It is important to use a full stop (period) «.» as a decimal separator, not a comma. The digestion volume is usually 20 mL, based on the usual digestion volume used in the procedure. Normally, there should be no difference between digestions of validation tests and regular measurements. However, depending on the weighed quantity, a higher digestion volume may be required for validation (e. g. 20 - 60 mL). Nevertheless, this is not covered here, as the aim is to calculate the MU of a regular sample and not the MU of validation tests.

Fall 3: Extraction

If the «Extraction» procedure was selected in the «Information on the procedure» section in the «Fundamentals» tab (see Figure 2), the measured value of the analyte is entered in box **22** after importing the model data and PDS, taking into account the concentration shown by the analytical device. If an internal standard is used, the latter is the concentration of that standard, e. g. milligrams per millilitre [mg/mL]. The correct units will be imported from the PDS. If a mean value has been determined, the two measured values are entered in boxes **22a - 22b** (see box **14** in section 2.1.3). Box **23** remains disabled (see Figure 6). Once calculation has taken place, it will contain the underlying measured values. If a second calibration is available in the PDS, that figure will be used for the determination of a mean value for the second entry in box **23**. If the figures in box **23** do not match those of the analysis device, it is possible that the analytical device has failed to take into account the increase in calibration variances (see discussion of the «Calculate» button, section 2.2).

In box **24**, the standard volume flow of the procedure is given in litres per minute [L/min] and in box **25** the standard sampling time of the procedure is given in minutes [min]. Box **26** remains disabled and is irrelevant for the «Extraction» procedure.

2.2.2 Result

Box **27** is selected to start calculating the measurement uncertainty for the data specified in section 2.2.1, «Validated Concentration». However, this is only possible if PDS data has been imported correctly and the model data has been confirmed.

The «Result» section comprises four further boxes, showing the result.

Box **29**: the calculated measured value β is the mass concentration.

Box **30**: u_c denotes the MU without the coverage factor. This is the combined standard uncertainty.

The extended MU of the procedure is calculated and reported in milligrams per cubic metre [mg/m^3] in box **31** and as a percentage in box **32**.

The right-hand column of the «Import-Calculate-Save» tab contains a table (see Figure 9). If «Calculate» (see box 27 in Figure 7) is clicked, to view all uncertainty percentages here with an influence on the measurement results. Note the following column names:

- «Influence» box **33**: Name of uncertainty parameter
- «Uncert.» box **34**: Calculated uncertainty of the parameter
- «SensCoeff.» box **35**: Calculated sensitivity coefficient
- «rel. Contrib.» box **36**: The relative percentage of the parameter in relation to the overall expected measurement uncertainty

2.3 Recovery

The imported recovery data is shown under this tab.

Figure 10: Imported recovery data (box 40 shows the table of imported data – not shown in this illustration due to insufficient column width: Temp1 and Temp2 follow after Hum2)

The «Recovery Data» section specifies the datasheet and PDS cells from which the data is being imported (see box **37** in Figure 10). Within IFA, only the data imported from the «Zusammenfassung MU» sheet are being considered.

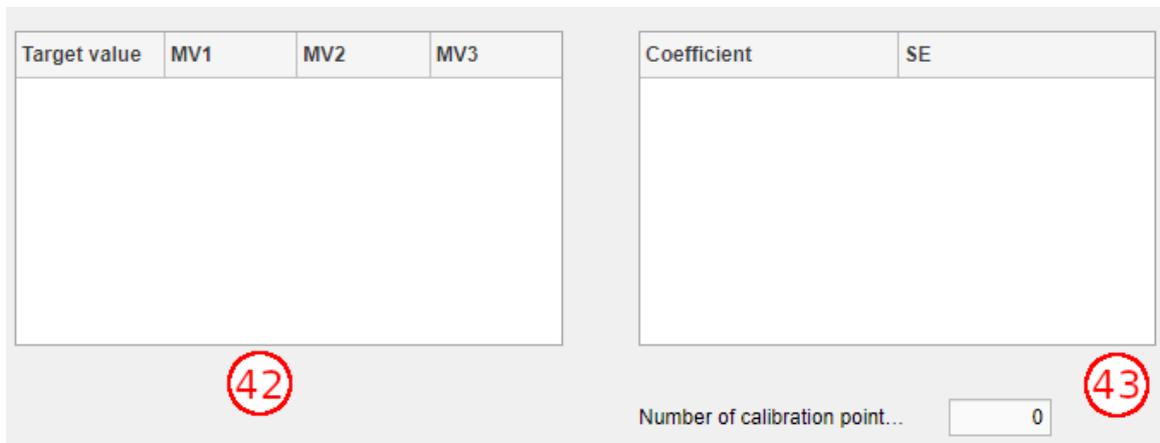
If the «Thermodesorption» or «Extraction» procedure is selected and if recovery data is available for the temperature and humidity (ticked and thus confirmed in boxes **10** under the «Fundamentals» tab, see Figure 3), then the app also uses the information from boxes **38** and **39** (see Figure 10). Otherwise they are disabled and of no relevance.

If the «Metals ICP-MS» procedure is selected, the app will only import recovery data under normal conditions, and the two boxes (**38**) and (**39**) remain disabled out and irrelevant. The table (see box **40**, Figure 10) shows the imported concentrations. Once they have been imported, they must be checked against the PDS. Conc. 1 - Conc. 6 specify concentrations under normal conditions (it is possible to place up to six different concentrations for recovery tests in the PDS). Hum1 - Hum2 each show the results of the recovery tests of three concentrations under a specified humidity. Temp1 - Temp2 each show the results of the recovery tests of three concentrations under a specified temperature.

Box **41**: By clicking «Calculate» in the «Import-Calculate-Save» tab, the table on the right (see Figure 10) will show the regression coefficients and their standard deviations as calculated for the weighted regression of the recovery tests. The purpose of the regression model is to calculate the uncertainty percentages for recovery. Underneath the table, the entire number of imported data items [N] underlying the regression model can be seen.

2.4 Calibration

This tab shows the imported calibration data from the PDS (see Figure 11). After data import, it should be verified with the PDS.



The screenshot displays a software interface for calibration data. It features two tables and a control field. The first table, labeled '42', has columns for 'Target value', 'MV1', 'MV2', and 'MV3'. The second table, labeled '43', has columns for 'Coefficient' and 'SE'. Below the second table is a text label 'Number of calibration point...' followed by a text input field containing the number '0'.

Target value	MV1	MV2	MV3
--------------	-----	-----	-----

Coefficient	SE
-------------	----

Number of calibration point...

Figure 11: Imported calibration data

Box **42**: The PDS can accommodate up to 3 measurements from the same calibration series. The app imports and stores all the data relating to calibration. The target value is the target concentration and measured values 1 - 3 specify the analysis values that go with the target values.

Box **43**: This table contains the calibration regression coefficients with their standard deviations. Underneath this table the entire number of imported calibration points (i. e. the basis of the regression model) is displayed. The purpose of the regression model is to calculate the uncertainty percentages of calibration. After importing the PDS, it should be checked if the number of calibration points is correct.

2.5 Model

The model data from the relevant Excel files are imported to this datasheet. The data forms the basis of a mathematical model for calculating β and U . There is no need to import this datasheet separately, as it is imported in parallel, along with the PDS, depending on the selected procedure. Further details of the here available data can be found in Chapter 3, «Model Datasheet».

Information	Indicator	Value	Procent	Description	Changed

44 46

45 Drift of analytical device 47 Sampling Head
- also changes flow rate -

Figure 12: Imported model data

This table contains the following details (see box **44** in Figure 12):

- Information: Abbreviation of uncertainty parameter
- Indicator: May have 1 or 2 as a value. Describes whether it is an absolute value, or whether the specified uncertainty value needs to be multiplied by the measured value.
- Value: The uncertainty contribution
- Percent: The specified uncertainty in percent, e. g. based on a standard, a calibration certificates, etc.
- Description: Description of the parameter

- Changed: Specifies whether the default value should be used (in which case the cell should be left empty) or whether a different value is used in the model (in which case the entry in this cell should be «changed»).

As specified in the list, each entry in the Model Datasheet has a default value. If the precise value for the measuring device drift of the analysis method is known, it can be changed via the menu (box **45**, see Figure 12). If the drift depends on the concentration, it needs to be adjusted for each calculation of the measurement uncertainty depending on the relevant concentration of the minimum measuring range. For example, if a lower drift value has been determined for low concentrations than the value for high concentrations, the lower value of the device drift needs to be entered for the calculation of the MU in the lower minimum measuring range, while using the higher value of the device drift for the calculation of the MU in the upper minimum measuring range. If the value is changed, «Use new entries» (box **46**) needs to be checked to accept those changes of the Model Datasheet (e. g. The device drift). The relevant entry in the table then changes, and the edits are noted in the «Changed» column. The button **46** does not need to be checked if there were no edits to any entries of the imported model data.

For methods involving samplers (metals/metalloids and particulates), either the details of the listed samplers from ISO 21832 or the individual estimators for the samplers concerning the sampling of respirable and inhalable dust from the same standard can be used.

Box 47: In the case of «Metals ICP-MS», with this menu it can be selected whether the sampler known for this procedure should be used for calculating the measurement uncertainty or the estimators of the sampling uncertainty components under ISO 21832.

3 Model Datasheet

All Model Datasheets can be found in an Excel file that comes with the app. Each procedure has its own datasheet, saved as an Excel datasheet within the same file.

3.1 Notes on Each Uncertainty Parameter

The uncertainty parameters are interpreted in the GUM as standard deviations. Not all stages of a validation have an influence on the measurement uncertainty. The following components must be covered in the calculations:

- Sampling
- Perhaps transportation of samples to the lab (only particulate substances, e. g. metals and metalloids)
- Sample preparation
- Calibration of measuring device(s)
- Recovery the substance
- Precision of measurement results upon comparison or repetition
- Drift of measuring devices
- Influence of temperature (for all except metals/metalloids, for gases and vapours, if the influence of the sampler is not known)
- Influence of humidity (for all except metals/metalloids)

The transportation of samples must only be covered if the upper limit of sample loss during transportation exceeds 5 %. However, it is generally assumed that sample loss during transportation is negligible.

The following validation components do not need to be covered:

- Transportation (except metals/metalloids)
- Storage (within the storage period, after a storage test)
- Detection and quantification limits
- Blank values

Storage can only be ignored if validation has shown that no storage-related loss of substance is likely to occur over a certain period of time.

3.1.1 Limits of Error

Manufacturers and standards specify most uncertainties in percentages. Such a percentage must be understood as a so-called limit of error. It means that the measurement result can only change, for instance, by $\pm 5\%$ in response to an influencing variable X . According to the principle of maximum entropy, it means that a random number that exists only within a fixed range can be described in terms of uniform distribution. The standard deviation estimate for a uniform distribution is half the width of the distribution range divided by $\sqrt{3}$. In this example, half the width is 5% of the measured value, i. e. $X \cdot 0,05$. The uncertainty would thus be calculated as follows:

$$s(X) = \frac{X \cdot 0.05}{\sqrt{3}} \quad (1)$$

In most cases (such as the above-mentioned limits of error), the measured value needs to be multiplied by the deviation or half the width of the distribution range (divided by either $\sqrt{3}$ or $\sqrt{6}$). In such cases, the Model Datasheet contains the indicator 2. If the indicator is 1, the value is an absolute value that does not require multiplication.

Specific examples and notes about the Model Datasheet are provided in the next few sections.

3.1.2 Thermodesorption

unit_beta is required for calculating β with the unit mg/m^3

unit_Vol is required for converting L to m^3 .

c_drift is the device drift, with 10% in the Model Datasheet by default. This value can be manually edited in the app. It is a limit of error for which the uncertainty level («value») can be calculated according to section 3.1.1 as follows:

$$s(c_{\text{drift}}) = \frac{c \cdot 0.1}{\sqrt{3}} \quad (2)$$

with c = output concentration/mass of the analysis device.

q_wdh is the repeatability uncertainty of the pump. Here, the worst-case value from Table B.1 in ISO 20581 with 2.3 % was used. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1).

$$s(q_{wdh}) = \frac{q \cdot 0.023}{\sqrt{3}} \quad (3)$$

where q = measured volume flow.

q_cal is the calibration uncertainty of the pump. Again, the worst-case value from Table B.1 in ISO 20581 with 5.2 % was used. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1):

$$s(q_{cal}) = \frac{q \cdot 0.052}{\sqrt{3}} \quad (4)$$

where q = measured volume flow.

q_stab is the uncertainty associated with the stability of the pump. The value was taken from ISO 13137 with 5 %. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1):

$$s(q_{stab}) = \frac{q \cdot 0.05}{\sqrt{3}} \quad (5)$$

where q = measured volume flow.

t_tot is the uncertainty associated with the measurement duration. It means working on the assumption that the «true» measurement duration differs from the defined measurement duration (e.g. standard sampling duration: two hours). It is assumed that the maximum deviation between the start and end of measurement is 0.5 min. As a result, a deviation of ± 1 min is applicable to the measurement procedure, and under ISO 22065 a triangular distribution is assumed in this instance. Accordingly, the uncertainty level («value») is calculated as follows:

$$s(t_{tot}) = \frac{1}{\sqrt{6}} \quad (6)$$

3.1.3 Metals ICP-MS

unit_calib is required for converting the unit of the calibration data from g to mg .

unit_beta is required for calculating β with the unit mg/m^3 .

unit_rec is required for converting the unit of the recovery data from g to mg .

unit_Vol is required for converting the volume from L to m^3 .

c_drift is the device drift, with 10 % in the Model Datasheet by default. This value can be manually edited in the app. It is a limit of error for which the uncertainty level («value») can be calculated according to section 3.1.1 as follows:

$$s(c_{\text{drift}}) = \frac{c \cdot 0.1}{\sqrt{3}} \quad (7)$$

with c = output concentration/mass in the analysis device.

q_wdh is the repeatability uncertainty of the pump. Here, the worst-case value from Table B.1 in ISO 20581 with 2.3 % was used. It is a limit of error for which the uncertainty level («value ») can be calculated as follows (see section 3.1.1):

$$s(q_{\text{wdh}}) = \frac{q \cdot 0.023}{\sqrt{3}} \quad (8)$$

where q = measured volume flow.

q_cal is the calibration uncertainty of the pump. Again, the worst-case value from Table B.1 in ISO 20581 with 5.2 % was used. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1):

$$s(q_{\text{cal}}) = \frac{q \cdot 0.052}{\sqrt{3}} \quad (9)$$

where q = measured volume flow.

q_stab is the uncertainty associated with the stability of the pump. The value was taken from ISO 13137 with 5 %. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1):

$$s(q_{\text{stab}}) = \frac{q \cdot 0.05}{\sqrt{3}} \quad (10)$$

where q = measured volume flow.

t_{tot} is the uncertainty associated with the measurement duration. It means working on the assumption that the «true» measurement duration differs from the defined measurement duration (e. g. standard sampling duration: two hours). It is assumed that the maximum deviation between the start and end of measurement is 0.5 min. As a result, a deviation of ± 1 min is applicable to the measurement procedure, and under ISO 22065 a triangular distribution is assumed in this instance. Accordingly, the uncertainty level («value») is calculated as follows:

$$s(t_{tot}) = \frac{1}{\sqrt{6}} \quad (11)$$

Uncertainties associated with volumes:

In the case of volumetric measuring devices, systematic and random deviations are mostly provided in calibration records or are determined during regular device qualification. The records contain the main deviations e_s which are required to add to or subtract from the volume (also later in the model). This adjustment influences the measurement results.

The following is usually applicable to the calculation of systematic errors associated with volumetric measuring devices:

$$s(V_{sys}) = \frac{z_s}{\sqrt{3}} \quad (12)$$

If only one volumetric measuring device is in use or if it is exactly known which one is in use, then $z_s = e_s$ which needs to be deducted from the reference volume. In such a case, calculation of the combined standard uncertainty would not involve a term for systematic deviation. However, most laboratory workplaces use a variety of volumetric devices, and it is difficult to trace which device was used to determine a specific reading. If a large number of pipettes is used on a daily basis and if their systematic deviation lies within a range of $\pm z_s$ around the measured value, then each measured value changes randomly within this range. This is similar to a limit of error, and such an influence is therefore treated as if it were a random effect.

The GUM does not rule out such a procedure (comment on 6.3.1 and F.2.4.5), if the extended measurement uncertainty is not increased across the board and to such an extent that it loses its informative value.

Uncertainties of volumetric measuring devices:

They include pipette uncertainties and dispensers (e. g. Hamilton). Individual labs often have a large number of pipettes. For this reason and also to reduce the amount of time spent on data updates, not all uncertainty values are saved for each pipette, but only the highest ones. To do so, all deviations of all pipettes, whether systematic or random, were pooled in advance for each test volume.

The individual pools were given an outlier test, and from the remaining pools, a pair consisting of the highest systematic deviation and the highest random deviation per test volume was selected for calculation within the app in each case.

V_0_rand_offen is the uncertainties associated with the reading error of the digestion solution after open digestion. Uncertainty is set at a relatively high value of 5 % and is influenced by calibration, manufacturer's specifications and the estimated individual error.

V_0_rand_MW is the uncertainties associated with the reading error after transferring the digestion solution of the microwave-assisted pressure digestion into the Falcon vessel. Uncertainty is set at a relatively high value of 10 % and is influenced by calibration, manufacturer's specifications and the estimated individual error.

V_1_rand1_10 is the random deviation of a pipette at a 1:10 dilution of the sample solution in the last step before analysis. The highest random uncertainty for this test volume is 0.85 %. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand1_10}) = \frac{V \cdot 0.0085}{\sqrt{3}} \quad (13)$$

Where V is the reference volume.

V_1_rand2_10 is the systematic deviation of a pipette at a 1:10 dilution of the sample solution in the last step before analysis. The highest random uncertainty for this test volume is 0.37 %. As described above, the systematic deviation is treated like a further random deviation. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand2_10}) = \frac{V \cdot 0.0037}{\sqrt{3}} \quad (14)$$

Where V is the reference volume.

V_1_rand1_100 is the random deviation of a pipette at a 1:100 dilution of the sample solution in the last step before analysis. The highest random uncertainty for this test volume is 0.54 %. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand1_100}) = \frac{V \cdot 0.0054}{\sqrt{3}} \quad (15)$$

Where V is the reference volume.

V_1_rand2_100 is the systematic deviation of a pipette at a 1:100 dilution of the sample solution in the last step before analysis. The highest random uncertainty for this test volume is 1.20 %. As described above, the systematic deviation is treated like a further random deviation. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand2_100}) = \frac{V \cdot 0.0120}{\sqrt{3}} \quad (16)$$

Where V is the reference volume.

V_1_rand1_1000 is the random deviation of a pipette at a 1:1000 dilution of the sample solution in the last step before analysis. The highest random uncertainty for this test volume is 0.83 %. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand1_1000}) = \frac{V \cdot 0.0083}{\sqrt{3}} \quad (17)$$

Where V is the reference volume.

V_1_rand2_1000 is the systematic deviation of a pipette at a 1:1000 dilution of the sample solution in the last step before analysis. The highest systematic uncertainty for this test volume is 4.48 %. As described above, the systematic deviation is treated like a further random deviation. The uncertainty level («value») is calculated as follows:

$$s(V_{1_rand2_1000}) = \frac{V \cdot 0.0448}{\sqrt{3}} \quad (18)$$

Where V is the reference volume.

V_st_rand1_10 is the random deviation of a volumetric measuring device (here: a dispenser) when adding the internal standard. The highest random deviation for this test volume is 0.12 %. The volume is the same for all levels of dilution. So, this is the deviation that is assumed for all dilutions. The uncertainty level («value») is calculated as follows:

$$s(V_{st_rand1_10}) = \frac{V \cdot 0.0012}{\sqrt{3}} \quad (19)$$

Where V is the reference volume.

V_st_rand2_10 is the systematic deviation of a volumetric measuring device (here: a dispenser) when adding the internal standard. The highest systematic deviation for this test volume is 1.42 %. The volume is the same for all levels of dilution. So, this is the deviation that is assumed for all dilutions. The uncertainty («Value») is calculated as:

$$s(V_{\text{st_rand2_10}}) = \frac{V \cdot 0.0142}{\sqrt{3}} \quad (20)$$

where V is the reference volume.

V_st_rand1_100 und 1000 in analogy with **V_st_rand1_10**.

V_st_rand2_100 und 1000 in analogy with **V_st_rand2_10**.

V_H2O_rand1_10 is the random deviation of the volumetric measuring device (here: the dispenser) when adding the dilution solution. The highest random deviation for this test volume is 0.003 %. The volume is the same for all levels of dilution. So, this is the deviation that we will assume for all dilutions. The uncertainty («Value») is calculated as follows:

$$V_{\text{H2O_rand1_10}} = \frac{V_{\text{H2O}} \cdot 0.00003}{\sqrt{3}} \quad (21)$$

V_H2O_rand2_10 is the systematic deviation of the volumetric measuring device (here: the dispenser) when adding the dilution standard. The highest systematic deviation for this test volume is 0.23 %. The volume is the same for all levels of dilution. So, this is the deviation that we will assume for all dilutions. The uncertainty («alue») is calculated as follows:

$$V_{\text{H2O_rand2_10}} = \frac{V_{\text{H2O}} \cdot 0.0023}{\sqrt{3}} \quad (22)$$

V_H2O_rand1_100 und 1000 in analogy with **V_H2O_rand1_10**.

V_H2O_rand2_100 und 1000 in analogy with **V_H2O_rand2_10**.

s_A/E: The app assumes that sampling systems generally comply with ISO 7708 and that there is **only one** uncertainty parameter for them. The relevant estimators are taken from ISO 21832 (C.3.4) and comprise several components. Depending on the fraction associated to the OELV selected in the «Fundamentals» tab, the app imports either the composite parameter for respirable dust sampling systems or for inhalable dust sampling systems.

For inhalable dust, the uncertainty parameter comprises the following components:

- Calibration of the sampler test system: 0.5 %
- Estimation of the sampled concentration: 4 %

- Bias relative to the sampling convention: 7.5 %

The uncertainty («Value») is calculated as follows:

$$s(s_E) = \frac{m \cdot 0.12}{\sqrt{3}} \quad (23)$$

where m is the mass on the filter.

For respirable dust, the uncertainty parameter comprises the following components:

- Calibration of the sampler test system: 1 %
- Estimation of the sampled concentration: 1 %
- Bias relative to the sampling convention: 8 %
- Flow excursion from the nominal flow rate for inertia-based pre-separators, e.g. cyclones and impactors:
 - when the sample volume is calculated from the nominal flow: 3 %, and when the sample volume is calculated from the average flow rate: 6 %.

- Individual sampler variability: 7 %.

The uncertainty («Value») is calculated as follows:

$$s(s_A) = \frac{m \cdot 0.23}{\sqrt{3}} \quad (24)$$

where m is the mass on the filter.

In both cases, it is possible to replace the one parameter with the individual sampler estimators for the sampling of respirable and inhalable dust derived from the same standard (see section 2.5, button **(46)**). As there are only the estimators from the standard, it is not possible to change the parameters for $s_{E/A}$ in the Model Datasheet. It is only possible to choose between the standard values using button **(46)** in the app.

3.1.4 Extraction

unit_beta is required for calculating β with the unit mg/m^3 .

unit_Vol is required for converting the volume from L to m^3 .

c_drift is the device drift, with 10 % in the Model Datasheet by default. This value can be manually edited in the app. It is a limit of error for which the uncertainty level («Value») can be calculated according to section 3.1.1, as follows:

$$s(c_{\text{drift}}) = \frac{c \cdot 0.1}{\sqrt{3}} \quad (25)$$

with c = output concentration/mass of the analytical device.

q_wdh is the repeatability uncertainty of the pump. Here, the worst- case value from Table B.1 in ISO 20581 was used, at 2.3 %. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1).

$$s(q_{\text{wdh}}) = \frac{q \cdot 0.023}{\sqrt{3}} \quad (26)$$

with q = measured volume flow.

q_cal is the calibration uncertainty of the pump. Again, the worst-case value from Table B.1 in ISO 20581 was used, at 5.2 % It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1).

$$s(q_{\text{cal}}) = \frac{q \cdot 0.052}{\sqrt{3}} \quad (27)$$

with q = measured volume flow.

q_stab is the uncertainty associated with the stability of the pump. The value was taken from ISO 13137, at 5 %. It is a limit of error for which the uncertainty level («value») can be calculated as follows (see section 3.1.1).

$$s(q_{\text{stab}}) = \frac{q \cdot 0.05}{\sqrt{3}} \quad (28)$$

with q = measured volume flow.

t_{tot} is the uncertainty associated with the measurement duration. It is assumed, that the «true» measurement duration differs from the defined measurement duration (e. g. standard sampling duration: two hours). It is further assumed that the maximum deviation between the start and end of measurement is 0.5 min. As a result, a deviation of ± 1 min is applicable to the measurement procedure, and under ISO 22065 a triangular distribution is assumed in this instance. Accordingly, the uncertainty («value») is calculated as follows:

$$s(t_{\text{tot}}) = \frac{1}{\sqrt{6}} \quad (29)$$

Uncertainties associated with volumes:

This covers the uncertainties of volumetric measuring devices (here: dispensers). All systematic deviations are treated as uniformly distributed random deviations (explanation see section 3.1.3).

Uncertainties of dispensers:

Individual labs often have many dispensers. For this reason and to reduce the amount of time spent on data updates, not all uncertainty values are saved for each dispenser, but only the highest uncertainty values. In order to that, all systematic and random deviations of all dispensers were pooled in advance for each test volume. The individual pools were subjected to an outlier test, and from the remaining pairs in the pools, a pair consisting of the highest systematic deviation and the highest random deviation per test volume was selected in each case in for calculation within the app.

V_{ex_rand1_2} is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 2 mL). The highest random deviation for this test volume is 0.09 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand1_2}}) = \frac{V \cdot 0.0009}{\sqrt{3}} \quad (30)$$

where V is the reference volume.

V_{ex_rand2_2} is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 2 mL). The highest random deviation for this test volume is 0.09 %. The uncertainty level («value ») is calculated as follows:

$$s(V_{\text{ex_rand2_2}}) = \frac{V \cdot 0.0033}{\sqrt{3}} \quad (31)$$

where V is the reference volume.

V_ex_rand1_2.5 is the systematic deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 2 mL). The highest random deviation for this test volume is 0.09 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand1_2.5}}) = \frac{V \cdot 0.0012}{\sqrt{3}} \quad (32)$$

where V is the reference volume.

V_ex_rand2_2.5 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 2.5 mL). The highest random deviation for this test volume is 0.12 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand2_2.5}}) = \frac{V \cdot 0.0031}{\sqrt{3}} \quad (33)$$

where V is the reference volume.

V_ex_rand1_3 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 3 mL). The highest random deviation for this test volume is 0.12 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand1_3}}) = \frac{V \cdot 0.0012}{\sqrt{3}} \quad (34)$$

where V is the reference volume.

V_ex_rand2_3 is the systematic deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 3 mL). The highest random deviation for this test volume is 0.31 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand2_3}}) = \frac{V \cdot 0.0031}{\sqrt{3}} \quad (35)$$

where V is the refernce volume.

V_ex_rand1_4 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 4 mL). The highest random deviation for this test volume is 0.25 %. The uncertainty level («value ») is calculated as follows:

$$s(V_{\text{ex_rand1_4}}) = \frac{V \cdot 0.0025}{\sqrt{3}} \quad (36)$$

where V is the reference volume.

V_ex_rand2_4 is the systematic deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 4 mL). The highest random deviation for this test volume is 0.53 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand2_4}}) = \frac{V \cdot 0.0053}{\sqrt{3}} \quad (37)$$

where V is the reference volume.

V_ex_rand1_5 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 5 mL). The highest random deviation for this test volume is 0.25 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand1_5}}) = \frac{V \cdot 0.0025}{\sqrt{3}} \quad (38)$$

where V is the reference volume.

V_ex_rand2_5 is the systematic deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 5 mL). The highest random deviation for this test volume is 0.53 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand2_5}}) = \frac{V \cdot 0.0053}{\sqrt{3}} \quad (39)$$

where V is the reference volume.

V_ex_rand1_10 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 10 mL). The highest random deviation for this test volume is 0.13 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand1_10}}) = \frac{V \cdot 0.0013}{\sqrt{3}} \quad (40)$$

where V is the reference volume.

V_ex_rand2_10 is the random deviation of the volumetric measuring device (here: a dispenser) when adding the extraction volume (in this case: 10 mL). The highest random deviation for this test volume is 0.13 %. The uncertainty level («value») is calculated as follows:

$$s(V_{\text{ex_rand2_10}}) = \frac{V \cdot 0.0043}{\sqrt{3}} \quad (41)$$

where V is the reference volume.

s_E: Mixtures of particles and vapour are exclusively sampling systems for inhalable dust in compliance with ISO 7708. In such cases, the app assumes that there is only one uncertainty parameter as detailed in ISO 21832 (C.3.4.1.2) and that it cannot be changed. It is composed as follows:

- Calibration of the sampler test system: 0.5 %
- Estimation of the sampled concentration: 4 %
- Bias relative to the sampling convention: 7.5 %:

The uncertainty level («value») is calculated as follows:

$$s(s_E) = \frac{m \cdot 0.12}{\sqrt{3}} \quad (42)$$

where m is the mass on the filter.

3.2 Editing uncertainty parameters

3.2.1 Filing Location of the Model Datasheet

The Model Datasheet can be found following the path

Messunsicherheit>v910>bin>win64.

The document is entitled «Modelldaten» (translated: «Model Data»). It is an Excel file in «xlsx» format.

3.2.2 Structure of the Model Datasheet

To create the mathematical model for the individual procedures, the app requires the Model Datasheet, which it imports together with the PDS. It does not need to be imported separately.

To ensure that the model data can be imported correctly, the datasheet must meet the following requirements:

- Title: «Modelldaten» (the title needs to be in German)
- File format: «.xlsx»
- Names of the subordinated data sheets: «Thermodesorption», «Metals», «Metalle», «Extraktion», «Extraction» (this is because the app is bilingual).

The app imports a range between cell B5 and cell G34 (area highlighted in yellow in the example file).

In addition, important is also the structure of the datasheet:

Column B: information

Column B contains the abbreviations of influencing factors under the heading of «information». The composition of the abbreviation is extremely important! The first letter indicates the measurand to which the influencing factor refers.

- c: output concentration / mass of the analytical device
- q: volume flowrate
- t: sampling duration
- V: volume
- s: mass on sample carrier (depending on sampler)

The underscore following the first letter forms the separator for further specifications, especially volumes. The following distinctions are made for factors influencing volumes:

- V_0: reading inaccuracy of digestion vessels
- V_1: uncertainties when transferring the aliquot
- V_st: uncertainties when adding the internal standard
- V_H2O: uncertainties when diluting the aliquot with ultrapure water
- V_ex: uncertainties when adding the extraction volume

The next underscore is a further separator.

It is followed by the specification whether the deviation is random or systematic.

- rand1: random deviation (e. g. specification in the calibration protocol: random deviation)
- rand2: systematic deviation that is to be treated like a random deviation (see section 3.1.3) (e. g. specification in the calibration protocol: systematic deviation)

After a further underscore as a separator, this is followed by the volume (for the extraction procedure) or the dilution factor (for the «Metals ICP-MS» procedure).

Column C: indicator

Column C, «indicator» is for a specifying indicator.

In most cases (such as limits of error), the multiplication of the measured value by the deviation or half the width of the distribution range (divided by either $\sqrt{3}$ or $\sqrt{6}$) is needed. In such cases, the assigned indicator in the Model Datasheet is 2. If the indicator is 1, the value is an absolute value that does not require multiplication.

Column D: value

Column D, «value», is for the calculated uncertainty. These are the uncertainties calculated with the equations (2) - (42).

Column E: percentage

Column E, «percentage», shows uncertainty percentages (e. g. limit of error) from specific sources (e. g. in literature). This serves the purpose of ensuring traceability to the values used.

Column F:

Column F contains plain text descriptions of the abbreviations and influencing factors listed in column B.

3.2.3 Editing Details in the Model Datasheet

In principle, it is possible to edit the Model Datasheet, provided that the structure of the datasheet as detailed in section 3.2.2, is not touched.

Case 1: Thermodesorption

Edits made to the Model Datasheet affect the influencing variables of the volume flowrate. If there have been tests on pump stability (repeatability uncertainty of the pump), the value of 2.3 % from ISO 20581 can be replaced. The same applies if any deviating values for pump stability or pump calibration are known. The drift of the analytical device can be adjusted directly in the app (**box 45**), see Figure 12. In addition, all descriptions in column F can be edited.

Case 2: Metals ICP-MS

As in case 1, the volume flow parameters can be edited, unless the worst-case values from standards ISO 20581 and ISO 13137 should be used. Both the datasheet and the app currently only allow three possible dilutions: 1:10, 1:100 and 1:1,000 (see **box 17**, Figure 4). Uncertainties can be edited in the datasheet if different deviations for the relevant volumetric measuring devices are known.

If one chooses different dilutions of the aliquot after the digestion of metallic substances, appropriate adjustments both in the Model Datasheet and in the app code must be made. In addition, all descriptions in column F can be edited.

Case 3: Extraction

As in cases 1 and 2, the volume flow parameters can be edited, unless the worst-case values from standards ISO 20581 and ISO 13137 should be used. Both the datasheet and the app so far only allow extraction volumes of 2 mL, 2.5 mL, 3 mL, 4 mL, 5 mL and 10 mL (see **box 13**, section 3). It is possible to edit the associated uncertainties in the datasheet if different deviations for the relevant volumetric measuring devices are known. Further extraction volumes can be added on request.

4 Instructions for Handling Error Messages

Table 3 lists all possible error messages, what they mean and what action is required when these messages appear.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Calibration not found	Either no calibration is available in the PDS or there is no cell link between the calibration Excel sheet and the «Zusammenfassung MU» datasheet. Import is incomplete, and the MU cannot be calculated	Check calibration data in the PDS.
Less than 3 calibration values	Either there are less than three calibration sets in the PDS or the cell link between the calibration Excel sheet and the «Zusammenfassung MU» datasheet is faulty. It is possible to calculate the MU based on two concentrations, but it is not very helpful and should be avoided.	Check calibration data in the PDS, complete to three calibration sets (after conducting outlier test in the PDS).
Regression of calibration is weighted	The calibration regression to determine the uncertainty is weighted because the variance is not constant. When analytical devices perform unweighted regression despite variable variance, deviations may occur between the app (box (23)) and the results of the analytical device.	Only for information. No action required.
Check calibration	There is at least one calibration point that only has one calibration value. Regression has been conducted unweighted although the variances are not constant. The calculated MU is not helpful. Only a program crash is prevented here.	Check calibration data in the PDS, complete to three calibration sets (after conducting outlier test in PDS).

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Outdated calibration with mean values	If only arithmetic mean values are available in PDS, then those values are used. This automatically leads to non-weighted regression, so that the associated variance is overestimated unless it is constant. A result is calculated even though this procedure should no longer be used.	There should be three measurements for each calibration point. Complete to three calibration sets.
Wrong unit or internal standard for thermodesorption.	At present, only thermodesorption methods without an internal standard are programmed in the app. Thus, no internal standard must be entered in the PDS (cell H3), and the only units that should be used here are either <i>[ng]</i> or <i>[mg]</i> . Measurement uncertainty is prevented from being calculated.	Check the PDS or choice of method.
Wrong unit or internal standard for extraction.	If an internal standard (box 12) has been selected, be sure to enter its concentration in cell H3 in the PDS. Otherwise, this cell should be vacant. Furthermore, the thermodesorption units (<i>[ng]</i> and <i>[mg]</i>) must not be entered as calibration units in the PDS (cell H4). Measurement uncertainty is prevented from being calculated.	Check the PDS or choice of method.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Wrong calibration unit (for ex- traction).	Cell H4 in the PDS on the «Zusammenfassung MU» datasheet contains either the unit of the internal stan- dard (if available) or the calibration unit (if there is no internal standard). The units of the supported mea- surement methods are: $[g/L]$, $[mg/mL]$, $[mg/L]$. Mea- surement uncertainty is prevented from being cal- culated.	Check the PDS or choice of method.
Wrong recovery unit (for ex- traction)	Cell H4 in the PDS on the (hidden) «Zusammenfas- sung MU» datasheet shows the unit of the recovery from method validation as a mass concentration in relation to an air volume. Permitted units: $[mg/m^3]$, $[g/m^3]$. Data import is stopped, and the measure- ment uncertainty cannot be calculated.	Check the PDS or choice of method.
Recovery not found.	There are no recovery data in the PDS. Either the wrong digestion method has been selected for «Met- als ICP-MS» in the «Fundamentals» menu, or the cell link from the recovery Excel datasheets to the «Zusammenfassung MU» datasheet is missing. Mea- surement uncertainty is prevented from being cal- culated.	Check recovery data in the PDS or pull-down menu (14) under «Fundamentals - Metals ICP- MS» for the correct digestion method. Alternatively, check the data of the recovery derived from the method validation in the PDS and, if necessary, compare with the (hidden) «Zusammen- fassung MU» datasheet.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Recovery: Less than 3 target concentrations	Either fewer than three target concentrations have been entered in the PDS for recovery or the cell link between the recovery Excel datasheets and the «Zusammenfassung MU» datasheet is missing. Measurement uncertainty is prevented from being calculated.	Check recovery data in the PDS and, if necessary, compare with (hidden) «Zusammenfassung MU» datasheet.
Recovery: Less than 6 repeat measurements	Either less than 6 repeat measurements have been entered per concentration in the PDS or the cell link between the recovery datasheets and the «Zusammenfassung MU» datasheet is incorrect. A calculation of measurement uncertainty is prevented for Metals ICP-MS and thermodesorption. For extraction, a calculation is possible but is accompanied by this warning.	Check recovery data in the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU» datasheet.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
<p>Recovery: Target concentrations missing</p>	<p>The target concentration has not been specified, although recovery data is available. Either there are no details in the PDS (datasheet «recovery» or «Extraction_Calibration&Recovery» or «Thermodesorption_Calibration&Recovery» or «Metals_Calibration&Recovery»), or the cell link between the recovery data and the «Zusammenfassung MU» datasheet is incorrect. The recovery data is ignored, which can distort the result. If ignoring such data leads to reduction of target concentrations to fewer than three, the calculation is prevented.</p>	<p>Check the humidity data in the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU» datasheet.</p>
<p>Humidity: Less than 6 repeat measurements</p>	<p>Humidity has been selected as a model component in box (10). Nevertheless, either less than 6 repeat measurements have been specified per concentration in the PDS or the cell link between the humidity datasheet and the «Zusammenfassung MU» datasheet is incorrect. Results are calculated which may be incorrect.</p>	<p>Check the humidity data in the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU» datasheet.</p>

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Humidity out of range	Humidity has been selected as a model component in box (10). Nevertheless, the details on low and high humidity in PDS, «Zusammenfassung MU» worksheet, do not comply with $20\% \pm 5\%$ and $80\% \pm 5\%$, as required. All values are assigned to either low or high humidity depending on their positions in the datasheet. This warning is displayed. Results are calculated which may be incorrect.	Check humidity details. If necessary, ensure that new measurements are taken.
Humidity: No target concentration	Humidity has been selected as a model component in box (10). Nevertheless, there is no specification of the target concentration for humidity tests, although recovery data is available. Either there are no details in the PDS (datasheet «recovery» or «Extraction_Calibration&Recovery» or «Thermodesorption_Calibration&Recovery» or «Metals_Calibration&Recovery»), or the cell link between the recovery data and the «Zusammenfassung MU» datasheet is incorrect. These data are ignored. Results are calculated which may be incorrect.	Check the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU» datasheet.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
No humidity data	Humidity has been selected as a model component in box (10). Nevertheless, either no recovery data for humidity is entered in the PDS, or the cell references between «Humidity» and the «Zusammenfassung MU» datasheet are incorrect. Results are calculated which may be incorrect.	Check humidity data and/or (hidden) datasheet «Zusammenfassung MU».
Temp.: Less than 6 repeat measurements.	Temperature has been selected as a model component in box (10). Nevertheless, either there are less than six repeat measurements for temperature during recovery in method validation in the PDS, or the cell references between the temperature tests worksheet and «Zusammenfassung MU» are incorrect. Results are calculated which may be incorrect.	Check temperature data in the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU Summary» datasheet.
Temperature not in the range	Temperature has been selected as a model component in box (10). Nevertheless, the details of low and high temperatures do not match those in the PDS, «Zusammenfassung MU» datasheet, as they are not $10 \pm 2^\circ\text{C}$ and $40 \pm 2^\circ\text{C}$, as required. This warning is displayed. All values are assigned to either low or high temperature depending on their positions in the datasheet. Results are calculated which may be incorrect.	Check temperature details. If necessary, ensure that new measurements are taken.

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Temp.: No target concentration	<p>Temperature has been selected as a model component in box (10). Nevertheless, there is no specification of the target concentration for humidity, although recovery data is available. Either there are no details in the PDS (datasheet «recovery» or «Extraction_Calibration&Recovery» or «Thermodesorption_Calibration&Recovery» or «Metals_Calibration&Recovery»), or the cell link between the recovery data and the «Zusammenfassung MU» datasheet is incorrect. Results are calculated which may be incorrect.</p>	<p>Check the PDS and, if necessary, compare with the (hidden) «Zusammenfassung MU» datasheet.</p>
No temperature data	<p>Temperature has been selected as a model component in box (10) in the PDS. Nevertheless, either the PDS does not contain any recovery data that include the temperature, or the cell references between «temperature» and the «Zusammenfassung MU» datasheet are incorrect. Results are calculated which may be incorrect.</p>	<p>Check temperature data in the PDS, «Extraction_Calibration&Recovery» or «Thermodesorption_Calibration&Recovery» or «Metals_Calibration&Recovery» or the (hidden) «Zusammenfassung MU» datasheet.</p>
Fit of recovery variance is linear	<p>Indicates the resulting dependence for the variances of the recovery values.</p>	<p>For information, no action required.</p>

Table 3: Descriptions of Possible Error Messages

Error message	Meaning	Required action
Fit of recovery variance is quadratic	Indicates the resulting dependence for the variances of the recovery values.	For information, no action required.
Take largest recovery variance	Indicates the resulting dependence for the variances of the recovery values.	For information, no action required.
Calibration for 2. column but no averaging	Calibration values have been entered for a second calibration even though box (14) «average» is not ticked. These calibration values are ignored. Results are calculated which may be incorrect.	Tick box (14), «average» or add just entry in the PDS.

5 Tool Version History

Version 1.0

This version has been available on the web site from September 2023 to October 2023 and is the initial version of the software. It contains models for the following processes:

- Measurement of the concentration of metals in the respirable or inhalable dust fraction using inductively coupled plasma mass spectrometry (ICP-MS). It is possible to provide data from two different digestion processes for the sampling material: open digestion as well as microwave-assisted digestion. The dilution factors are: 10, 100, 1000.
- Measurement of the analyte after extraction using chromatographic methods (high performance liquid chromatography (HPLC) or gas chromatography (GC)). The analytes may be sampled from particulate-vapour mixtures or from gases/vapours. It is possible to use internal standards for calibration and measurement. One may also average the results of two columns. In this case it is possible to account for separate calibrations. The following extraction volumes are available: 2 mL, 2.5 mL, 3 mL, 4 mL, 5 mL, 10 mL.
- Measurement of volatile analytes after thermodesorption using gas chromatography.

Version 1.1

This version has been available on the web site from October 2023 to February 2024 and resolves an error in the calculation of the uncertainty with respect to the random part of the recovery. The respective standard deviation is estimated from the variances of the recovery measurements under repeatability conditions at each nominal value. Version 1.1 calculates now the standard deviation for a given measured value (analyte) at the corresponding nominal value. If the slope in the recovery model is close to 1, the deviations to the preceding versions are small.

Version 1.2

This version is available since February 2024 and resolves an error in the calculation of the sensitivity coefficient of the uncertainty with respect to the random part of the recovery. The uncertainty term is now correctly added to the nominal value of the concentration or mass and not to the measured value. If the slope in the recovery model is close to 1, the deviations are small.

6 References

ISO 7708: Air quality - Particle size fraction definitions for health-related sampling (01/1996). Berlin, Beuth Verlag GmbH.

ISO 21832: Workplace air - Metals and metalloids in airborne particles - Requirements for evaluation of measuring procedures (08/2020) Berlin. Beuth Verlag GmbH.

ISO/IEC GUIDE 98-3: Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (1995). Genf, Schweiz.

DIN EN 482: Workplace exposure - Procedures for the determination of the concentration of chemical agents - Basic performance requirement (05/2021) Berlin, Beuth Verlag GmbH.

ISO 20581: Workplace air - General requirements for the performance of procedures for the measurement of chemical agents (11/2016) Genf, Schweiz

TRGS 402: Technische Regeln für Gefahrstoffe - Ermitteln und Beurteilen der Gefährdungen bei Tätigkeiten mit Gefahrstoffen: Inhalative Exposition (2016), GmBl. Köln, Carl Heymanns Verlag

ISO 13137: Workplace atmospheres - Pumps for personal sampling of chemical and biological agents - Requirements and test methods (01/2023) Genf, Schweiz

ISO 22065: Workplace air - Gases and vapours - Requirements for evaluation of measuring procedures using pumped samplers (11/2020) Genf, Schweiz