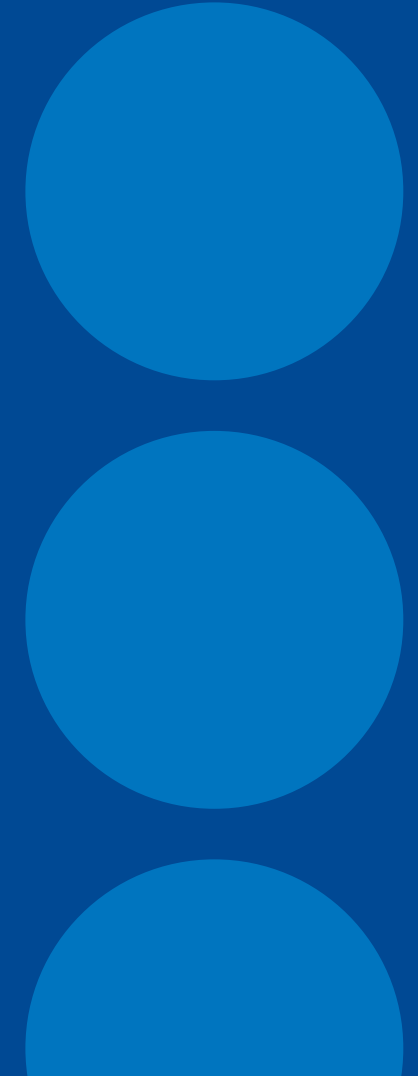


“MUST“ – A tool for the determination of measurement uncertainty and more

PEROSH, September 8th 2023

Dr. Cornelia Wippich, cornelia.wippich@dguv.de

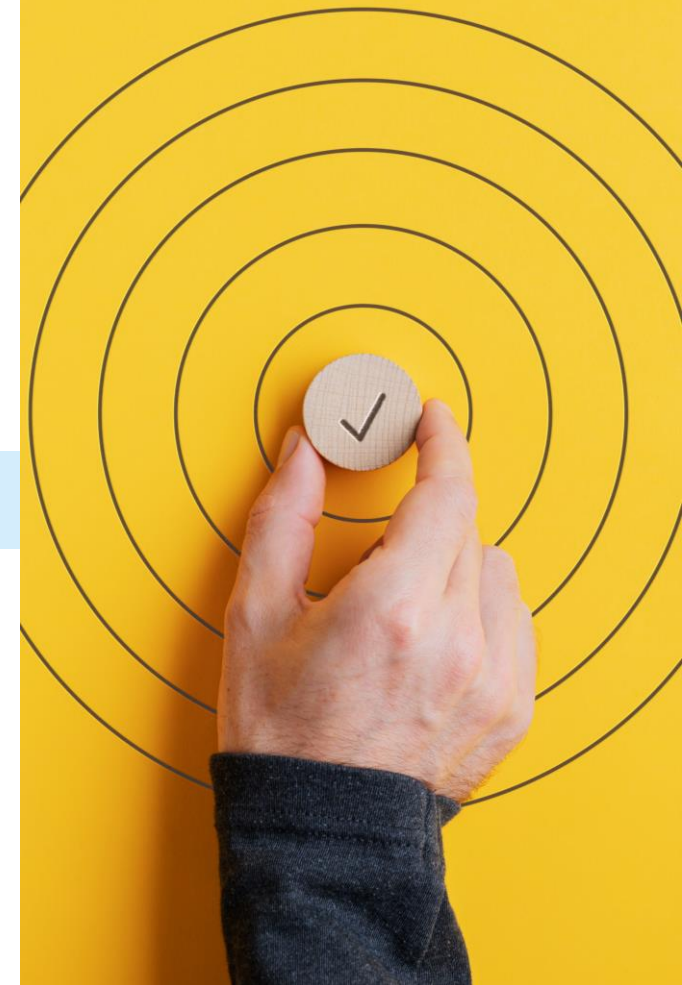


- True value is unknown
- Measurement value is an estimate influenced by factors
- The uncertainty:
 - parameter associated with the result to a measurement
 - characterized by the variance contributed to a measurement parameter

Why do we need measurement uncertainty?

- Customer request
- Legal regulation (comparison to OELV)
- Accreditation (ISO 17025)
- Comparison with other laboratories and improvement of the measurement method

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Standards, Regulations and Sources



ISO/IEC Guide 98-3 Uncertainty of measurement – Part 3: Guide to the expression of uncertainty in measurement (GUM)



EN 482:2021 Workplace exposure – Procedures for the determination of the concentration of chemical agents – basic performance requirements



ISO 20581:2016 Workplace air – General requirements for the performance of procedures for the measurement of chemical agents



ISO 21832:2020 Workplace air – Metals and metalloids in airborne particles – Requirements for evaluation of measuring procedures



ISO 22065:2021 Workplace air – Gases and vapours – Requirements for evaluation of measuring procedures using pumped samplers



ISO 23861: Workplace air - Chemical agent present as a mixture of airborne particles and vapour - Requirements for evaluation of measuring procedures

Basic requirements to measurement uncertainty

According to EN 482 and ISO 20581

Minimum measuring ranges

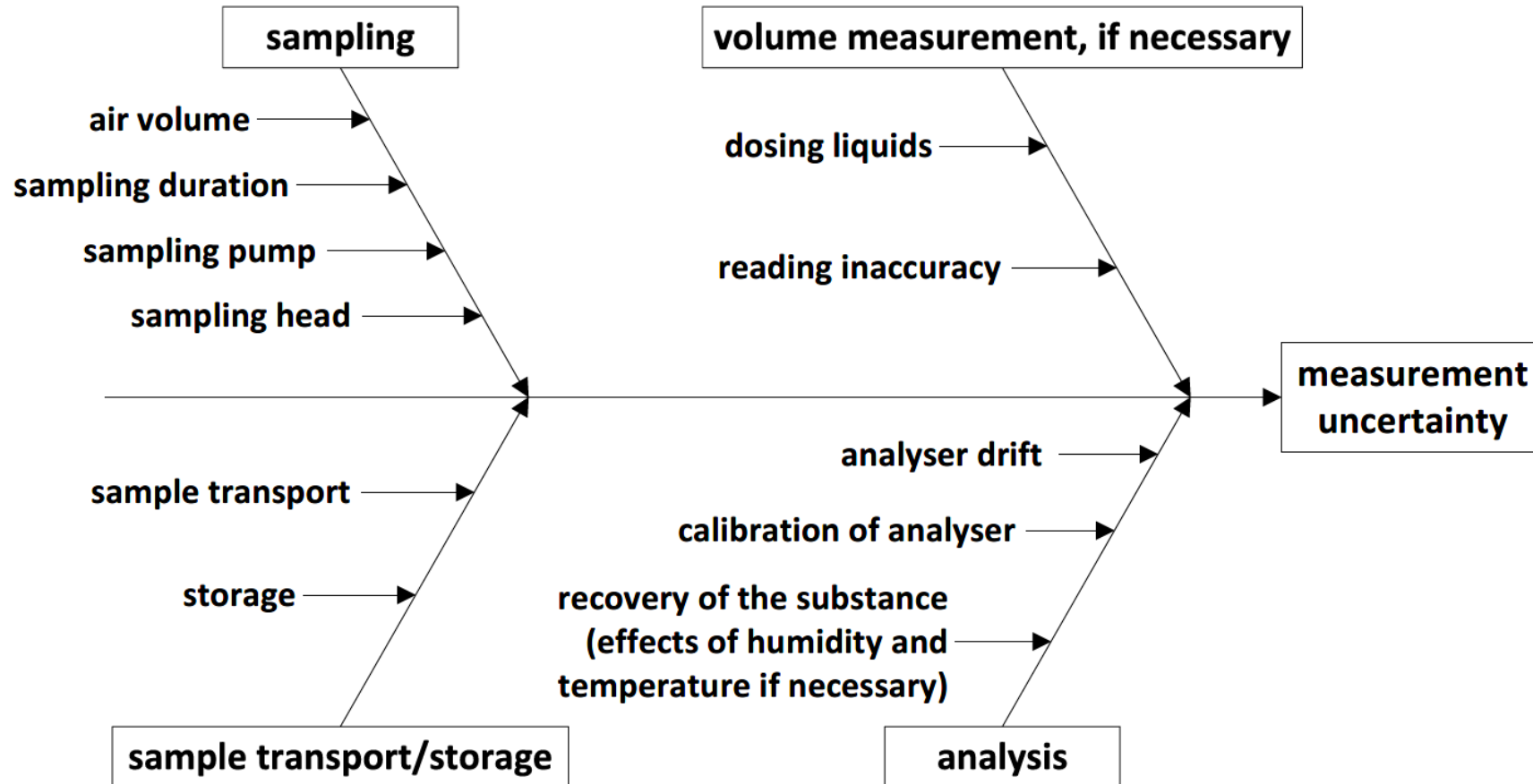
- Health-based limit values (shift average): 0.1 – 2 LV
- Risk-based limit values (in Germany): 0.2 AK (acceptable risk) – 2 TK (tolerable risk)

Expanded measurement uncertainty (U) for the measurement method:

- $U \leq 50\%$ 0.1 – 0.5 LV (0.2 AK – 1 AK)
- $U \leq 30\%$ 0.5 – 2 LV (1 AK – 2 TK)
- $U \leq 50\%$ for mixtures of particles and vapor



What data is required?

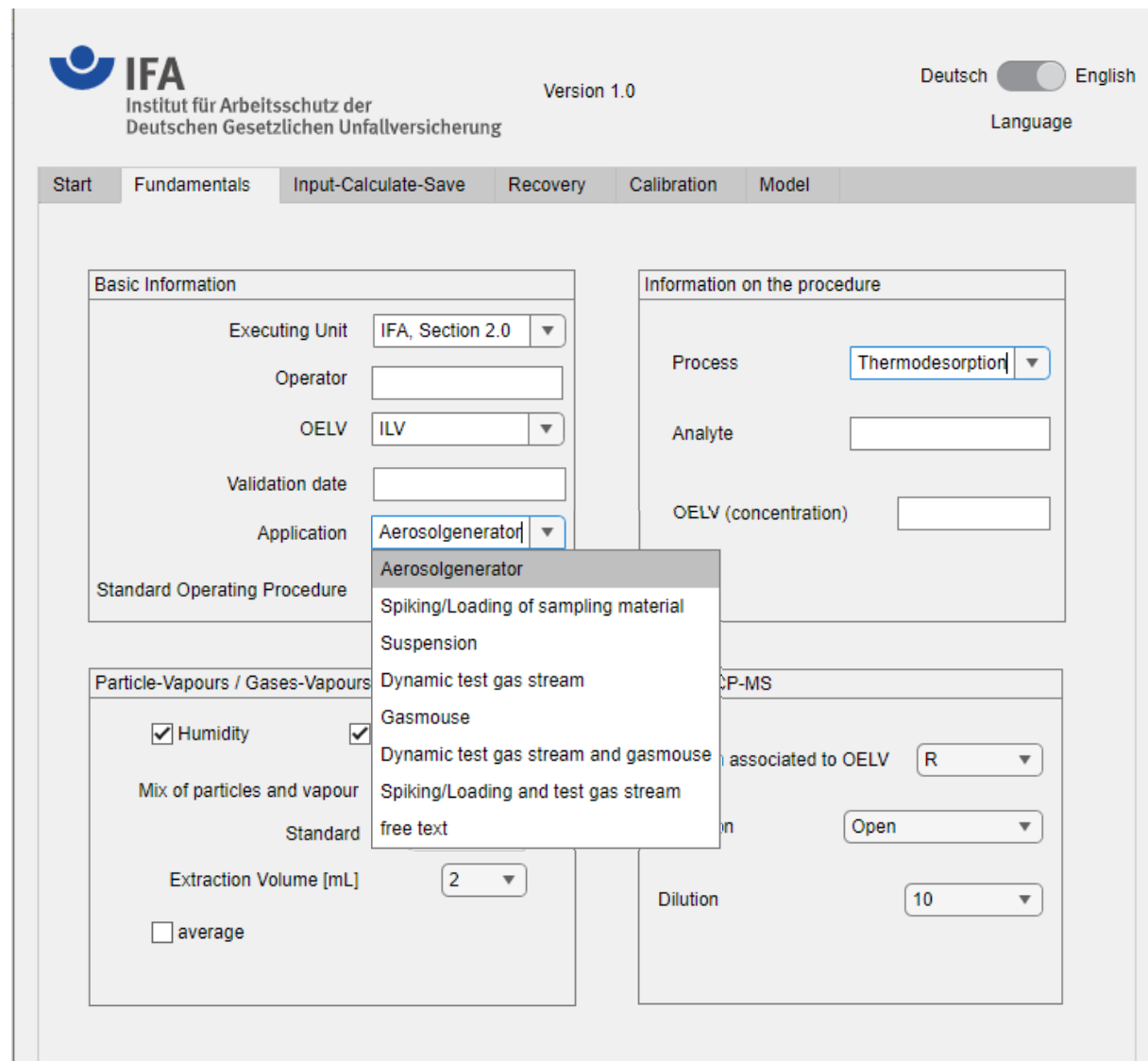


MUST - The measurement uncertainty service tool

Basic Information

- Information on validation / person / date
- Type of OELV
- Application

Extraction/Thermodesorption or Metals with ICP-MS



The screenshot shows the MUST software interface with the following details:

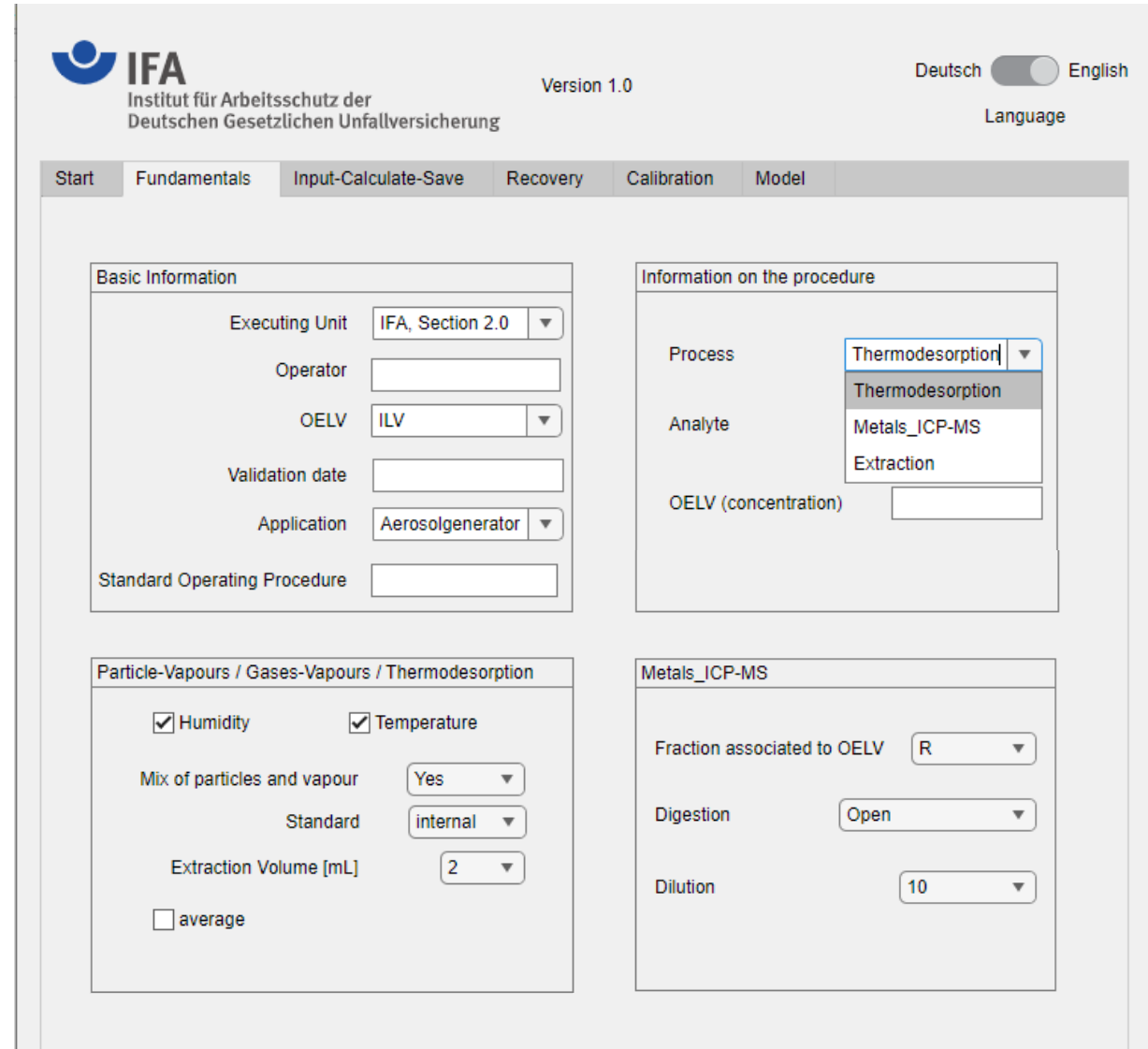
- Header:** IFA logo, Institut für Arbeitsschutz der Deutschen Gesetzlichen Unfallversicherung, Version 1.0, Deutsch/English language toggle.
- Tabs:** Start, Fundamentals, **Input-Calculate-Save**, Recovery, Calibration, Model.
- Basic Information:**
 - Executing Unit: IFA, Section 2.0
 - Operator: [text input]
 - OELV: ILV
 - Validation date: [text input]
 - Application: Aerosolgenerator
- Information on the procedure:**
 - Process: Thermodesorption
 - Analyte: [text input]
 - OELV (concentration): [text input]
- Standard Operating Procedure:**
 - Aerosolgenerator (selected)
 - Spiking/Loading of sampling material
 - Suspension
 - Dynamic test gas stream
 - Gasmouse
 - Dynamic test gas stream and gasmouse
 - Spiking/Loading and test gas stream
 - free text
- Particle-Vapours / Gases-Vapours:**
 - Humidity:
 - Mix of particles and vapour:
 - Standard: [text input]
 - Extraction Volume [mL]: 2
 - average:
- ICP-MS:**
 - associated to OELV: R
 - [text input]
 - Open: [text input]
 - Dilution: 10

MUST - The measurement uncertainty service tool

Basic Information

Procedure / Method

- Method (3 different types to chose from)
- Analyte (documentation)
- OELV (documentation)
- Depending on method
- Extraction: humidity/temperature if necessary; volume
- Metals: sampling head, digestion method, dilution factor



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Version 1.0

Deutsch English
Language

Start Fundamentals **Input-Calculate-Save** Recovery Calibration Model

Basic Information

Executing Unit: IFA, Section 2.0

Operator:

OELV: ILV

Validation date:

Application: Aerosolgenerator

Standard Operating Procedure:

Information on the procedure

Process: Thermodesorption

Analyte: Metals_ICP-MS

OELV (concentration):

Particle-Vapours / Gases-Vapours / Thermodesorption

Humidity Temperature

Mix of particles and vapour: Yes

Standard: internal

Extraction Volume [mL]: 2

average

Metals_ICP-MS

Fraction associated to OELV: R

Digestion: Open

Dilution: 10

MUST - The measurement uncertainty service tool




1 Data provision

- Load data

Influence factors

Concentration

Result of calculation



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Version 1.0

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Language

Start
Fundamentals
Input-Calculate-Save
Recovery
Calibration
Model

Data provision

Get data
Show Error Messages

Recovery

Calibration

Accept Model

Validated concentration

Analyte [mg/L]

Measured value dimensionless

Flow rate [L/min]

Sampling duration [min]

Digestion volume [mL]

Calculate
Save

Result

beta [mg/m³]

u_c

U [mg/m³]

U [%]

Influence	Uncert.	SensCoeff.	rel. Contrib.
Recovery (rand)	6.4e-02	6.4e-03	1.2
Recovery (sys)	2.1e-02	6.7e-03	0.1
Calibration	2.7e-01	6.4e-03	20.6
Humidity	4.0e-02	6.4e-03	0.5
Temperature	0.0e+00	6.4e-03	0.0
Ambient conditions	8.7e-03	-1.1e-01	5.9
Volume internal standard	1.4e-06	1.6e+01	0.0
Drift of analytical devices	2.9e-01	6.4e-03	23.4
Repetition (pump)	1.3e-04	-3.2e+00	1.2
Calibration (pump)	3.0e-04	-3.2e+00	6.3
Stability (pump)	2.9e-04	-3.2e+00	5.9
Sampling duration	4.1e-01	-1.1e-03	1.3
Dispenser extraction vo...	1.0e-06	1.6e+01	0.0
Dispenser extraction vo...	3.8e-06	1.6e+01	0.0
ISO 21832 - Sum I	6.6e-04	3.3e+00	33.7

MUST - The measurement uncertainty service tool

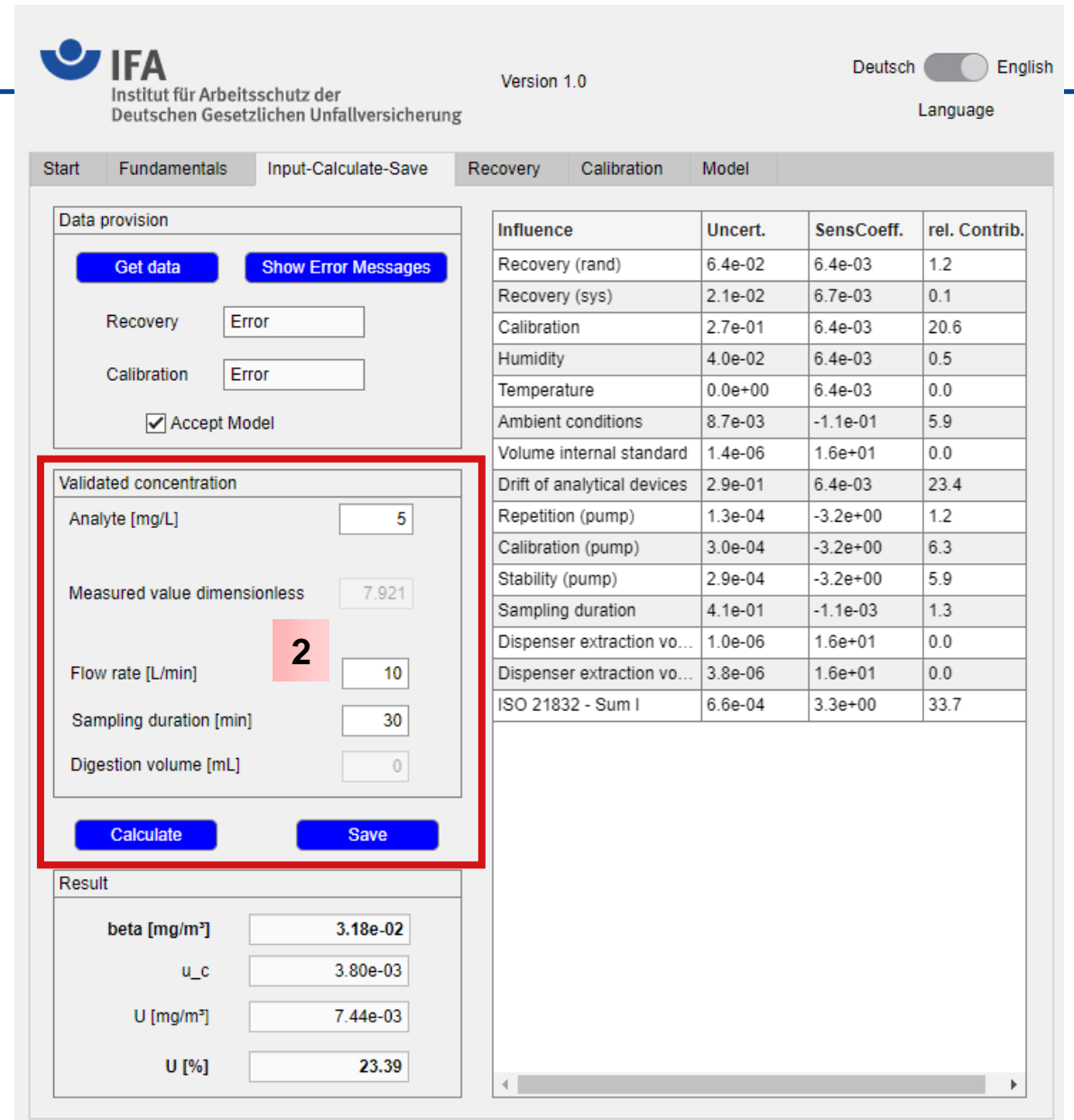


Data provision

2 Concentration

Parameters of measurement or validation
Influence factors

Result of calculation



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Language

Start Fundamentals **Input-Calculate-Save** Recovery Calibration Model

Data provision

Get data Show Error Messages

Recovery Error

Calibration Error

Accept Model

Validated concentration

Analyte [mg/L] 5

Measured value dimensionless 7.921

Flow rate [L/min] 2 10

Sampling duration [min] 30

Digestion volume [mL] 0

Calculate Save

Result

beta [mg/m³] 3.18e-02

u_c 3.80e-03

U [mg/m³] 7.44e-03

U [%] 23.39

Influence	Uncert.	SensCoeff.	rel. Contrib.
Recovery (rand)	6.4e-02	6.4e-03	1.2
Recovery (sys)	2.1e-02	6.7e-03	0.1
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Dispenser extraction vo...	3.8e-06	1.6e+01	0.0
ISO 21832 - Sum I	6.6e-04	3.3e+00	33.7

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Data provision


Concentration

3 Influence Factors

- Factors

Result of calculation

ent



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Language

Start
Fundamentals
Input-Calculate-Save
Recovery
Calibration
Model

Data provision

Get data
Show Error Messages

Recovery

Calibration

Accept Model

Validated concentration

Analyte [mg/L]

Measured value dimensionless

Flow rate [L/min]

Sampling duration [min]

Digestion volume [mL]

Calculate
Save

Result

beta [mg/m³]

u_c

U [mg/m³]

U [%]

Influence	Uncert.	SensCoeff.	rel. Contrib.
Recovery (rand)	6.4e-02	6.4e-03	1.2
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ISO 21832 - Sum I	6.6e-04	3.3e+00	33.7

3

MUST - The measurement uncertainty service tool



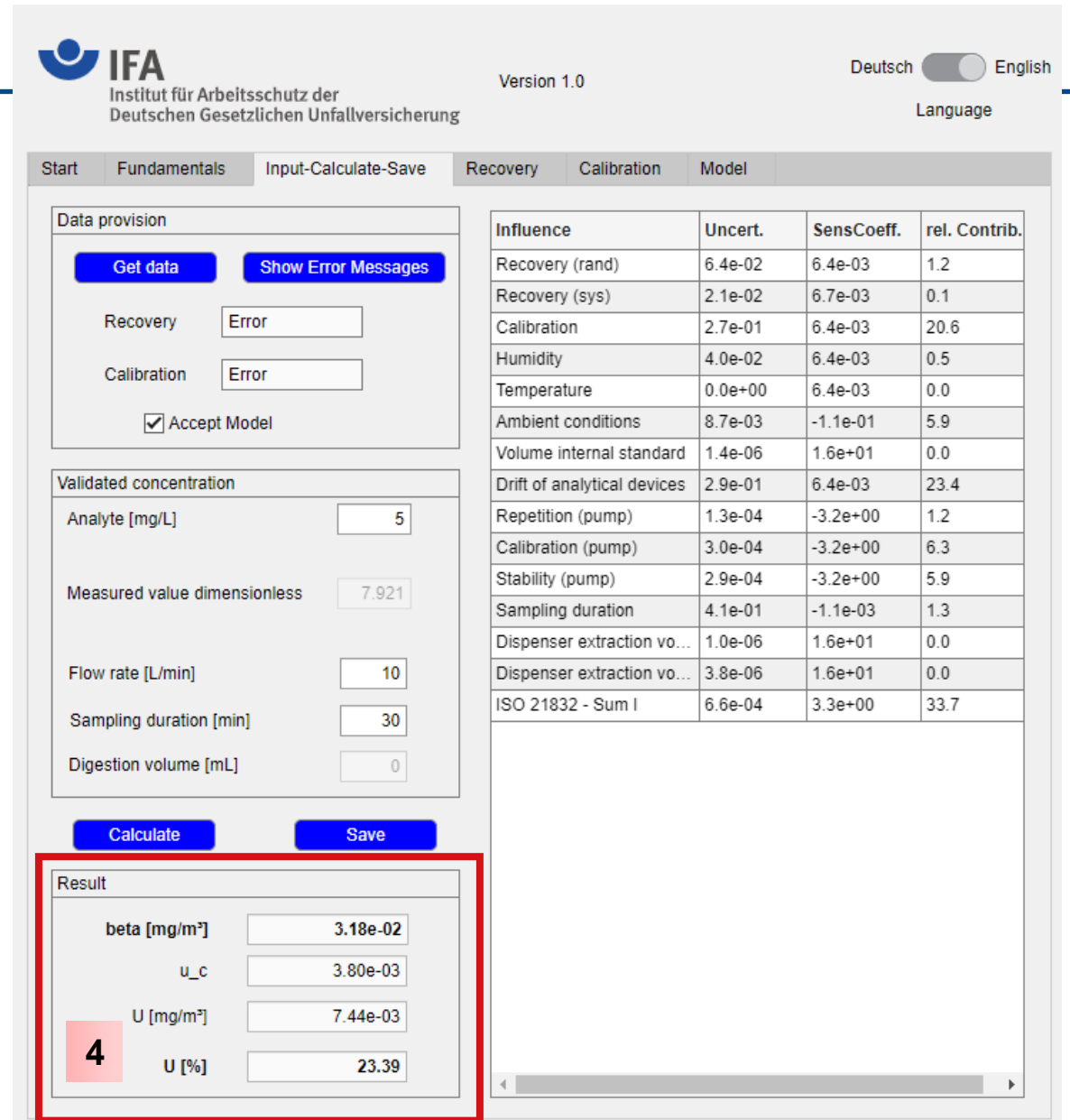
Data provision

Influence factors

Concentration

4 Result of calculation

- β : corrected measurement value
- u_c : combined standard uncertainty
- U : expanded measurement uncertainty



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Start Fundamentals Input-Calculate-Save Recovery Calibration Model

Data provision

Get data Show Error Messages

Recovery Error

Calibration Error

Accept Model

Validated concentration

Analyte [mg/L] 5

Measured value dimensionless 7.921

Flow rate [L/min] 10

Sampling duration [min] 30

Digestion volume [mL] 0

Calculate Save

Result

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Temperature	0.0e+00	6.4e-03	0.0
Ambient conditions	8.7e-03	-1.1e-01	5.9
Volume internal standard	1.4e-06	1.6e+01	0.0
Drift of analytical devices	2.9e-01	6.4e-03	23.4
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Sampling duration	4.1e-01	-1.1e-03	1.3
Dispenser extraction vo...	1.0e-06	1.6e+01	0.0
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ISO 21832 - Sum I	6.6e-04	3.3e+00	33.7

Recovery

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Start Fundamentals Input-Calculate-Save Recovery Calibration Model

Recovery data

Influence factor	Tab Name	Sections
Recovery normal conditions	Zusammenfassung MU	A19:F32
	Zusammenfassung MU	H19:M31
	Zusammenfassung MU	O19:T31

	Coefficient	SE
b_0	-0.0000	0.0000
b_1	1.0526	0.0040
b_H	-0.0074	0.0036
b_T	0	0

Amount of data N: 48

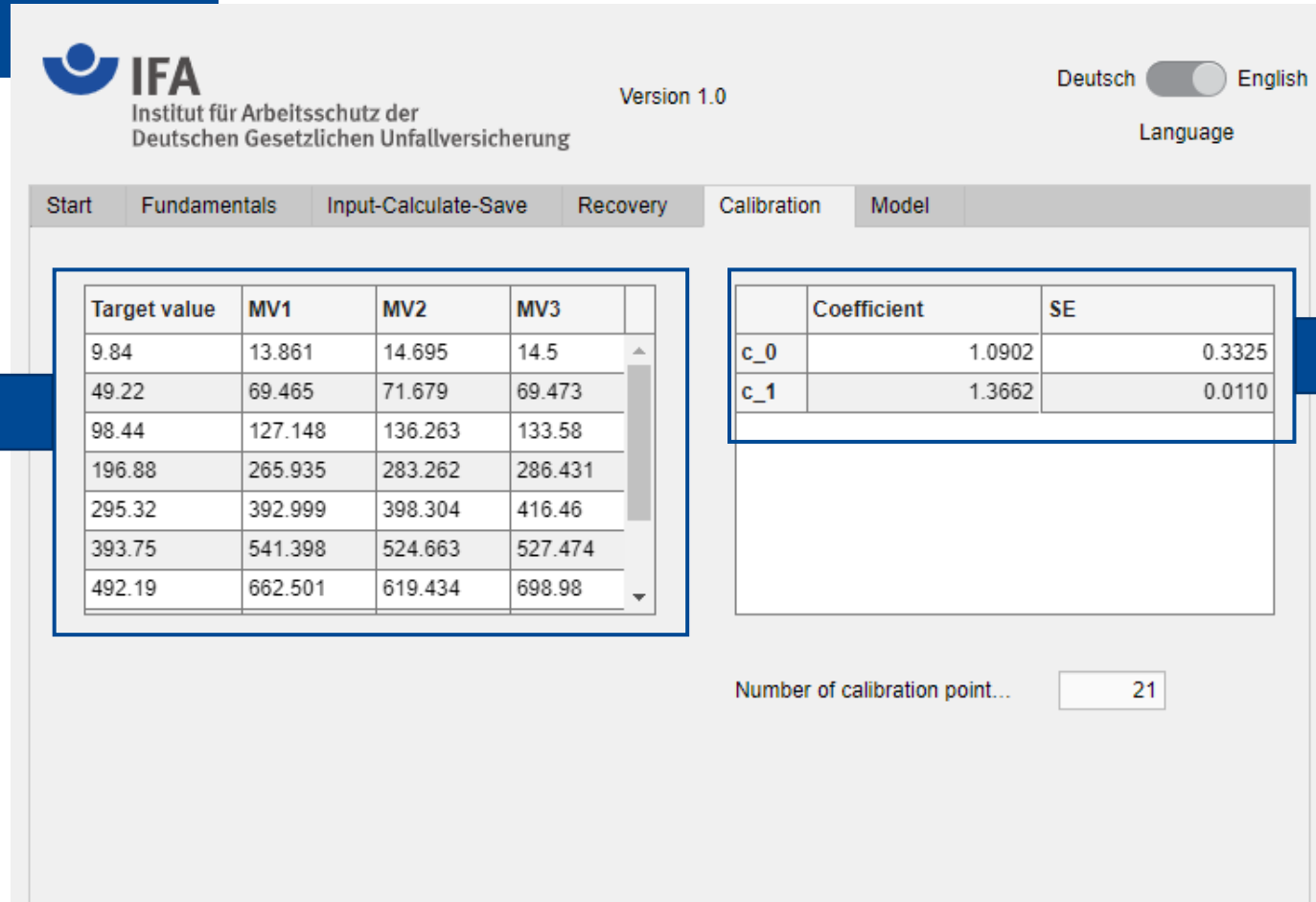
	Conc. 1	Conc. 2	Conc. 3	Conc. 4	Conc. 5	Conc. 6	Hum1	Hum1
Target-concentration	19.1	47.5	198.1				19	19.1
Unit	µg/m³	µg/m³	µg/m³	µg/m³	µg/m³	µg/m³	µg/m³	µg/m³
	19.239	50.145	214.005				20.326	20.326
	19.501	49.69	210.95				20.258	20.258
	19.245	50.032	212.336				20.308	20.308
	19.516	49.649	207.206				19.976	19.976
	19.417	49.998	209.606				20.341	20.341
	19.447	50.176	208.29				20.259	20.259

source

measurement values

regression coefficients

Calibration



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Start Fundamentals Input-Calculate-Save Recovery Calibration Model

Target value	MV1	MV2	MV3
9.84	13.861	14.695	14.5
49.22	69.465	71.679	69.473
98.44	127.148	136.263	133.58
196.88	265.935	283.262	286.431
295.32	392.999	398.304	416.46
393.75	541.398	524.663	527.474
492.19	662.501	619.434	698.98

	Coefficient	SE
c_0	1.0902	0.3325
c_1	1.3662	0.0110

Number of calibration point...

calibration
data

regression
coefficients

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Model Datasheet

- Name of parameter
- Value of uncertainty with sensitivity coefficient
- Percent as given in standards or other sources (changeable)
- Description

Start Fundamentals Input-Calculate-Save Recovery Calibration Model

	Information	Indicator	Value	Procent	Description
1	unit_beta		1		equals mg/m ³
2	unit_Vol		0.001		l in m ³
3	c_drift	2	5.77350269189625814e-02	10	Drift of analytical devices
4	q_wdh	2	1.32790561913613929e-02	2.3	Repetition (pump)
5	q_cal	2	3.00222139978605397e-02	5.2	Calibration (pump)
6	q_stab	2	2.88675134594812907e-02	5	Stability (pump)
7	t_tot	1	4.08248290463863073e-01		Sampling duration
8	V_ex_rand1_2	2	5.19615242270663239e-04	0.09	Dispenser extraction volume (ranc
9	V_ex_rand2_2	2	1.90525588832576517e-03	0.33	Dispenser extraction volume (sys)
10	V_ex_rand1_2.5	2	6.92820323027550913e-04	0.12	Dispenser extraction volume (ranc
11	V_ex_rand2_2.5	2	1.78978583448783984e-03	0.31	Dispenser extraction volume (sys)
12	V_ex_rand1_3	1	5e-06		Dispenser extraction volume (ranc
13	V_ex_corr_3	1	-5e-06		Dispenser extraction volume (sys)
14	V_ex_rand1_4	2	1.44337567297406449e-03	0.25	Dispenser extraction volume (ranc
15	V_ex_corr_4	1	-2.04e-05	0.53	Dispenser extraction volume (sys)
16	V_ex_rand1_5	2	1.44337567297406449e-03	0.25	Dispenser extraction volume (ranc
17	V_ex_rand2_5	2	3.05995642670501677e-03	0.53	Dispenser extraction volume (sys)
18	V_ex_rand1_10	2	7.50555349946513471e-04	0.13	Dispenser extraction volume (ranc
19	V_ex_rand2_10	2	2.48260615751539097e-03	0.43	Dispenser extraction volume (sys)
20	s_l	2	0.069282	12	ISO 21832 - Sum l

Use new entries

Drift of analytical device

Sampling Head

- also changes flow rate -

Required Datafiles

- “MUST” (.exe) can be downloaded from IFA-website for free:
<https://mustdownload.ifa.dguv.de/>
- Download is about 2.5 GB (background: MATLAB runtime environment);
folder includes datasheets for validation data
- User manual (GER/ENG) will follow in September 2023 at the website:
<https://www.dguv.de/ifa/praxishilfen/hazardous-substances/software-must/index.jsp>
- Help, Support and questions:
must@dguv.de



Thanks for the attention!

