University of Stuttgart
Germany
Institute for Sanitary Engineering,
Water Quality and Solid Waste Management
AQS Baden-Württemberg

INTERNATIONAL STANDARD **ISO 11352**

First edition
2012-07-01

Water quality — Estimation of measurement uncertainty based on validation and quality control data

Qualité de l'eau — Estimation de l'incertitude de mesure basée sur des données de validation et de contrôle qualité

Uncertainty estimation according to ISO 11352 using MS EXCEL®

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Background of ISO 11352:2012

- is based on the 2nd edition of the NORDTEST TR 537
- focused on „Water quality“ because it was developed by the ISO TC 147 “Water quality“
- revision probably starts in 2023

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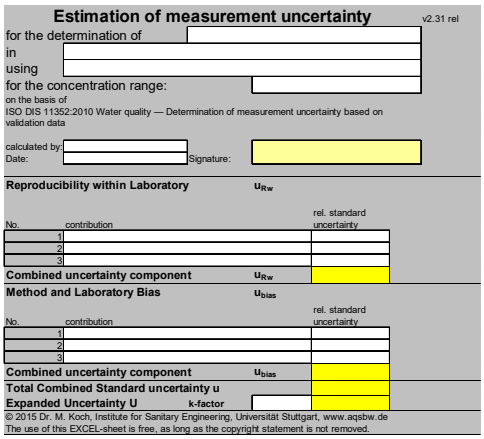
The Excel tool

- aims to
  - mirror ISO 11352 as closely as possible
  - provide laboratories with an easy-to-use tool
  - serve as a documentation for the mu estimation



Estimation of measurement uncertainty v2.31 rel

for the determination of
in
using
for the concentration range:
on the basis of
ISO DIS 11352:2010 Water quality — Determination of measurement uncertainty based on validation data

calculated by:
Date: Signature:

Reproducibility within Laboratory u_{Rw}

No.	contribution	rel. standard uncertainty
1		
2		
3		

Combined uncertainty component u_{Rw}

Method and Laboratory Bias u_{bias}

No.	contribution	rel. standard uncertainty
1		
2		
3		

Combined uncertainty component u_{bias}

Total Combined Standard uncertainty u

Expanded Uncertainty U k-factor

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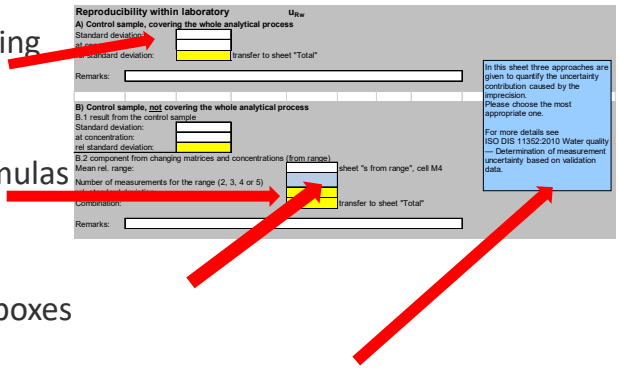
Basics on the tool

- white cells are for entering data
- yellow cells contain formulas
- blue cells are selection boxes
- blue text boxes are for information
- the sheets are protected, but without password, allowing the user to make individual adjustments



Reproducibility within laboratory u_{Rw}

A) Control sample, covering the whole analytical process

Standard deviation:
at c
rel standard deviation:
transfer to sheet "Total"

Remarks:

In this sheet three approaches are given to quantify the uncertainty contribution caused by the imprecision.
Please choose the most appropriate one.

For more details see ISO DIS 11352:2010 Water quality — Determination of measurement uncertainty based on validation data.

B) Control sample, not covering the whole analytical process

B.1 result from the control sample
Standard deviation:
at concentration:
rel standard deviation:

B.2 component from changing matrices and concentrations (from range)
Mean rel. range:
sheet "s from range", cell M4
Number of measurements for the range (2, 3, 4 or 5)
Combination:
transfer to sheet "Total"

Remarks:

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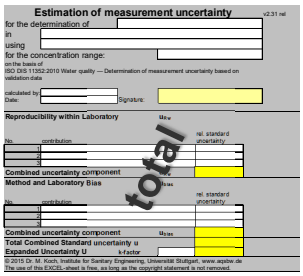
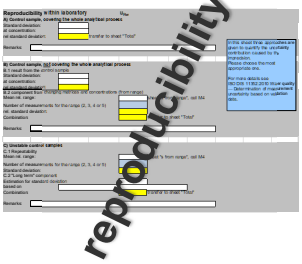
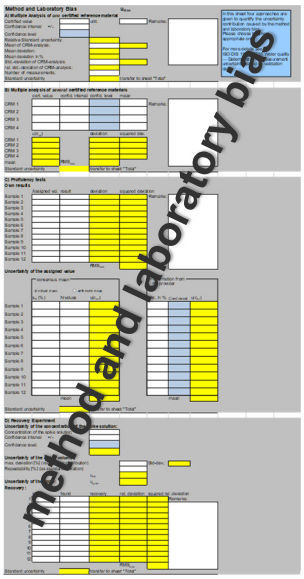
Main sheets of the tool



Intended for summarising the results and used as cover of the documentation



Data and calculations on the precision part



Data and calculations on the trueness part

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Sheet „total“ - I

Estimation of measurement uncertainty v2.31 rel

for the determination of
in
using
for the concentration range:
on the basis of
ISO DIS 11352:2010 Water quality — Determination of measurement uncertainty based on validation data

calculated by:
Date: Signature:

- Specification of the measurand
- Possibility to sign the printed document

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Sheet „total“ - II

Reproducibility within Laboratory	u_{Rw}	
No.	contribution	rel. standard uncertainty
1		
2		
3		
Combined uncertainty component	u_{Rw}	
Method and Laboratory Bias	u_{bias}	
No.	contribution	rel. standard uncertainty
1		
2		
3		
Combined uncertainty component	u_{bias}	
Total Combined Standard uncertainty u		
Expanded Uncertainty U	k-factor	

- final result will be here
- Summary of precision and trueness part

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Sheet „reproducibility“

Reproducibility within laboratory u_{Rw}

A) Control sample, covering the whole analytical process
Standard deviation:
at concentration:
rel standard deviation: transfer to sheet "Total"

Remarks:

In this sheet three approaches are given to quantify the uncertainty contribution caused by the imprecision.
Please choose the most appropriate one.

For more details see ISO DIS 11352:2010 Water quality — Determination of measurement uncertainty based on validation data.

B) Control sample, not covering the whole analytical process
B.1 result from the control sample
Standard deviation:
at concentration:
rel standard deviation:
B.2 component from changing matrices and concentrations (from range)
Mean rel. range: sheet "s from range", cell M4
Number of measurements for the range (2, 3, 4 or 5)
rel. standard deviation:
Combination: transfer to sheet "Total"

Remarks:

C) Unstable control samples
C.1 Repeatability
Mean rel. range: sheet "s from range", cell M4
Number of measurements for the range (2, 3, 4 or 5)
Standard deviation:
C.2 "Long term" component
Estimation for standard deviation based on
Combination: transfer to sheet "Total"

Remarks:

8.2.2 Control samples covering the whole analytical process

$$u_{R_w} = s_{R_w}$$

8.2.3 Using standard solutions as quality control samples

$$u_{R_w} = \sqrt{u^2_{R_w,stand} + u^2_{r,range}}$$

$u_{r,range}$: calculated from mean range

8.2.4 Unstable control samples

$$u_{R_w} = \sqrt{u^2_{r,range} + u^2_{R_w,bat}}$$

$u_{R_w,bat}$: variations between batches, e.g. from scientific judgement

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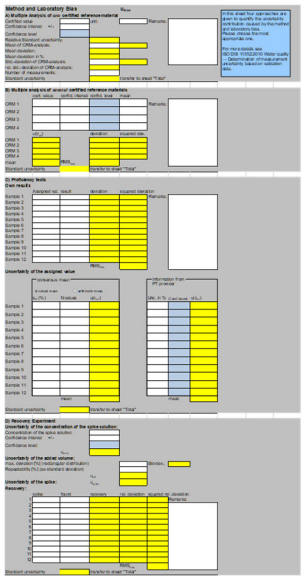
Sheet „method and laboratory bias“



one reference material

several reference materials

interlaboratory comparisons

recovery experiments

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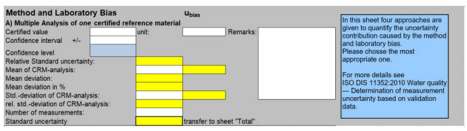
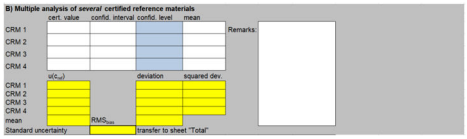
Sheet „method and laboratory bias“

8.3.2 Analysis of suitable reference materials



one reference material

$$u_b = \sqrt{b^2 + \left(\frac{s_b}{\sqrt{n_M}}\right)^2 + u_{C_{ref}}^2}$$



several reference materials

$$u_b = \sqrt{\bar{u}_{C_{ref}}^2 + b_{rms}^2}$$

with

$$b_{rms} = \sqrt{\frac{\sum(b_i)^2}{n_r}}$$

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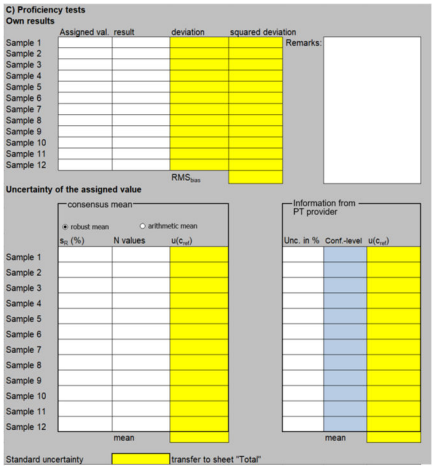
Sheet „method and laboratory bias“

8.3.3 Participation in interlaboratory comparisons


C) Proficiency tests
Own results
Assigned val. result deviation squared deviation
Sample 1 … Sample 12
Remarks:
RMS$_{bias}$
Uncertainty of the assigned value
consensus mean
robust mean arithmetic mean
$s_{R,i}$ (%) N values $u(c_{ref})$
Information from PT provider
Unc. in % Conf.-level $u(c_{ref})$
mean mean
Standard uncertainty transfer to sheet "Total"

own results

$$D_{rms} = \sqrt{\frac{\sum(D_i)^2}{n_{ilc}}}$$

uncertainties of the assigned values

- from PT provider information or
- calculated for consensus values

$$u_{C_{ref},i} = \frac{s_{R,i}}{\sqrt{n_{p,i}}} \text{ or}$$

$$u_{C_{ref},i} = 1.25 \times \frac{s_{R,i}}{\sqrt{n_{p,i}}}$$

finally $u_b = \sqrt{\bar{u}^2_{C_{ref}} + D^2_{rms}}$

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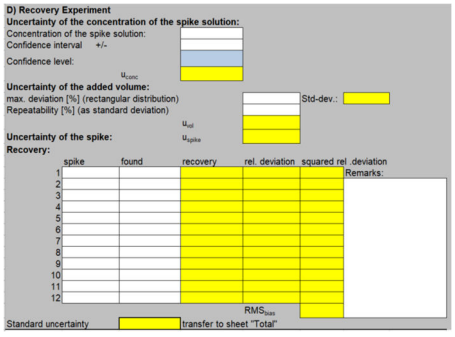
Sheet „method and laboratory bias“

8.3.4 Recovery experiments


D) Recovery Experiment
Uncertainty of the concentration of the spike solution:
Concentration of the spike solution:
Confidence interval +/-
Confidence level:
u_{conc}
Uncertainty of the added volume:
max. deviation [%] (rectangular distribution)
Repeatability [%] (as standard deviation)
Std-dev.:
u_{rel}
Uncertainty of the spike: u_{spike}
Recovery:
spike found recovery rel. deviation squared rel. deviation
Remarks:
1 … 12
RMS$_{bias}$
Standard uncertainty transfer to sheet "Total"

uncertainties of the spiking

- concentration u_{conc}, e.g. from a certificate
- added volume

$$u_V = \sqrt{u^2_{V,b} + u^2_{V,rep}}$$

- and thus $u_{add} = \sqrt{u^2_V + u^2_{conc}}$

recovery $b_{rms} = \sqrt{\frac{\sum(b_i)^2}{n_\eta}}$

and finally $u_b = \sqrt{b^2_{rms} + u^2_{add}}$

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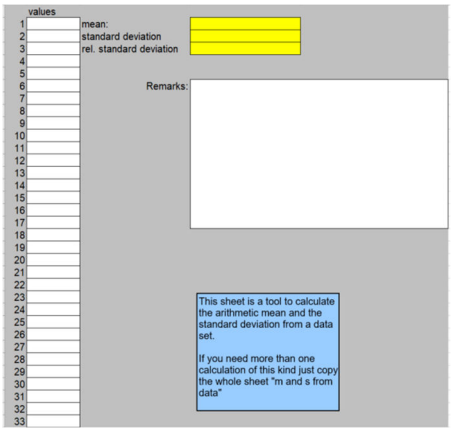
Auxiliary sheet „m and s from data“



- simple tool to calculate arithmetic mean, standard deviation and relative standard deviation from a set of data

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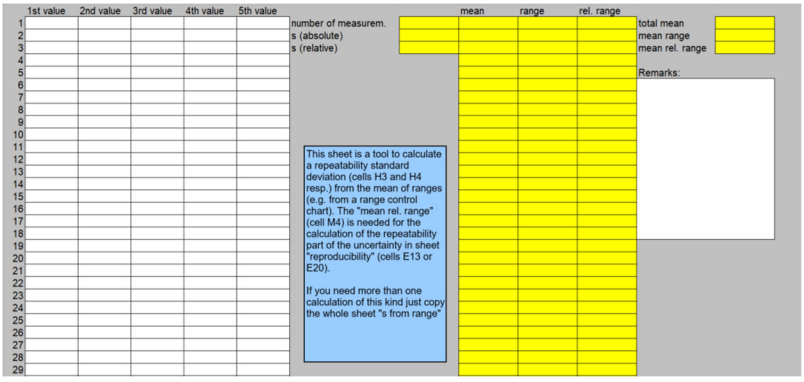
Auxiliary sheet „s from range“



- tool to calculate the mean range and mean rel. range of a set of replicated results as a basis to calculate the repeatability standard deviation (Annex A)

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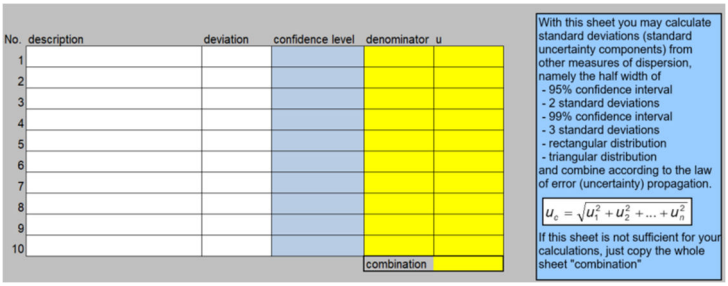
Auxiliary sheet „combination“



No.	description	deviation	confidence level	denominator	u
1					
2					
3					
4					
5					
6					
7					
8					
9					
10					
				combination	

With this sheet you may calculate standard deviations (standard uncertainty components) from other measures of dispersion, namely the half width of
- 95% confidence interval
- 2 standard deviations
- 99% confidence interval
- 3 standard deviations
- rectangular distribution
- triangular distribution

and combine according to the law of error (uncertainty) propagation.

$$u_c = \sqrt{u_1^2 + u_2^2 + \ldots + u_n^2}$$

If this sheet is not sufficient for your calculations, just copy the whole sheet "combination"

- can be used if there is a need to calculate the square root of the sum of squares of several contributions „uncertainty propagation“

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Summary

- The tool 1:1 reproduces the standard ISO 11352:2012
- There are two versions, one to calculate mu in quantity units, one to calculate relative mu – both versions in German and in English
- For more details on the calculation please consult the standard
- This tool is quite popular in Germany and available from www.aqsbw.de/en

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Thank you very much!

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