

## Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

Eurachem Workshop – Uncertainty from sampling and analysis  
for accredited laboratories  
19.-20. November 2019, Berlin

Steffen Uhlig  
Kirsten Simon  
Bertrand Colson  
Karina Hettwer  
Kirstin Frost



### Introduction

Amendment of the Federal Soil Protection and Contaminated Sites Ordinance



- Current draft of Federal Soil Protection and Contaminated Sites Ordinance (May 2017)
  - Use of the term **uncertainty of results** instead of **uncertainty of measurement**
  - Recommendations concerning the permissible uncertainty of results of procedures and methods are given by the Expert Advisory Board for Soil Investigations (FBU).
  - No *general* definition of result uncertainties, since possibly contaminated sites may differ considerably from case to case with respect to the distribution of contaminants.
    - **Determination of the uncertainty of results on a case by case basis**
- No harmonized procedure for taking into account measurement uncertainty in the conformity assessment of measurement results (i.e. with respect to trigger and action values)
- In a research project funded by the Federal Environment Agency (Umweltbundesamt), harmonized guidelines for enforcement authorities were developed.

## Introduction

Amendment of the Federal Soil Protection and Contaminated Sites Ordinance



- Environmental Research Plan of the Federal Ministry for the Environment, Nature Conservation, Construction and Nuclear Safety (UFOPLAN 3715 74 299 0)
- Guide for the implementation of the Federal Soil Protection and Contaminated Sites Ordinance provides guidance for taking measurement uncertainty into account in the conformity assessment of measurement results.

- PD Dr. habil. Steffen Uhlig, Dipl.-Math Henning Baldauf,  
Dipl.-Math Kirstin Frost, Dr. Karina Hettwer,  
Dipl.-Psych. Kirsten Simon (MBA)  
QuoData GmbH, Quality & Statistics!, 01309 Dresden
- Dr. Frank Küchler, Sampling,  
15345 Rehfelde OT Werder
- Prof. Dr. mult. Dr. h. c. Konstantin Terytze,  
Federal Environment Agency,  
Expert Advisory Board for Soil Investigations,  
06844 Dessau-Roßlau

Handlungsanleitung zum Umgang mit der Ergebnisunsicherheit bei der Über- und Unterschreitung von Prüf- und Maßnahmenwerten für den Vollzug der Bundes-Bodenschutz- und Altlastenverordnung

Umweltforschungsplan des  
Bundesministeriums für Umwelt,  
Naturschutz, Bau- und Verkehrssicherheit  
UFOPLAN 3715 74 299 0  
U0619/00

Handlungsanleitung zum Umgang mit der Ergebnisunsicherheit bei der Über- und Unterschreitung von Prüf- und Maßnahmenwerten für den Vollzug der Bundes-Bodenschutz- und Altlastenverordnung

Autoren:

Prof. Dr. habil. Steffen Uhlig<sup>1)</sup>,

Dipl.-Math. Henning Baldauf<sup>1)</sup>,

Dipl.-Math. Kirstin Frost<sup>1)</sup>,

Dr. Karina Hettwer<sup>1)</sup>,

Dipl.-Psych. Kirsten Simon (Master of Business Administration)<sup>2)</sup>,

<sup>1)</sup> QuoData GmbH, Quality & Statistics!, 01309 Dresden

Dr. Frank Küchler, Beratung/Praxisfirma, 15345 Rehfelde OT Werder

<sup>2)</sup> Prof. Dr. habil. Dr. h. c. Konstantin Terytze, Umweltbundesamt, Fachbereich für Bodenuntersuchungen, 06844 Dessau-Roßlau

Ansprechpartner:

Prof. Dr. habil. Steffen Uhlig, QuoData GmbH, Quality & Statistics!, Postfach 14,  
01309 Dresden, Tel. +49 (0) 351 40 20 867/0, Fax +49 (0) 351 40 20 867/20

Im Auftrag des Umweltbundesamtes

Januar 2019

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de

3

## Conceptual framework

Measurement uncertainty components



- A conceptual framework for the calculation of measurement uncertainty in connection with the implementation of the Federal Soil Protection and Contaminated Sites Ordinance has been developed.
- The following measurement uncertainty components are taken into consideration:
  - (1) uncertainty due to **spatial heterogeneity** of contaminants in the site / area
  - (2) uncertainty due to **sampling**
    - systematic errors
    - random errors
  - (3) uncertainty due to **fundamental variability**,
  - (4) uncertainty due to **chemical analysis**
    - systematic errors
    - random errors
- These measurement uncertainty components represent all uncertainty sources whose inclusion is required by the German Accreditation Body GmbH (DAkkS).

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de

4

## Conceptual framework

### Measurement uncertainty components



#### (1) Spatial heterogeneity

- Spatial heterogeneity reflects the circumstance that contaminant loads are not uniformly distributed throughout a given site, i.e. there are locations with higher or lower contaminant loads within the site.

#### (2) Sampling

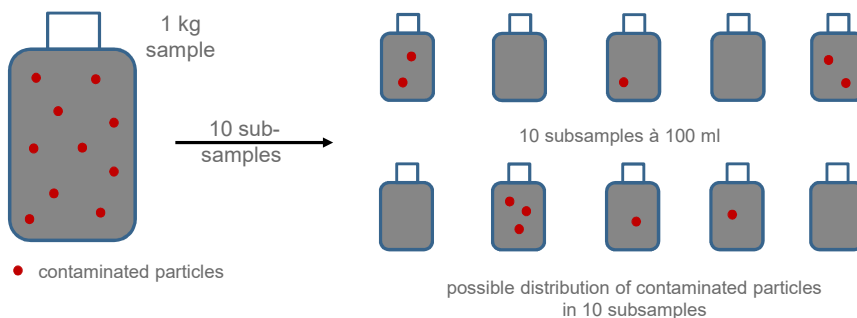
- Includes uncertainty contributions which arise in connection with sampling procedures, sample packaging, sample preservation and transport.
- For calculation of the sampling uncertainty a concentration-dependent variance model is applied. Information from sampling interlaboratory tests is taken into consideration.

## Conceptual framework

### Measurement uncertainty components



#### (3) Fundamental variability



- Fundamental variability reflects the fact that for each subsample the number of contaminated particles as well as their analyte content is subject to random variation, even if the material is perfectly homogenized.
- For the calculation of the fundamental variability, simulations are performed with contaminant concentration, particle size and sample volume as parameters

## Conceptual framework

### Measurement uncertainty components



#### (4) Analytical method

- This component includes uncertainties arising from sample pretreatment, preparation and processing, and from contaminant detection and quantification.
- For the calculation of systematic and random deviations, different options are available: (1) use of PT data, (2) applying a concentration-dependent variance model, or (3) usage of the Horwitz standard deviation.

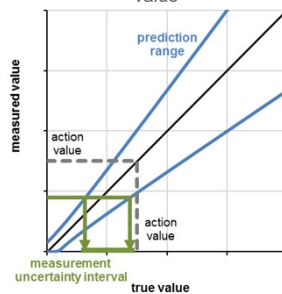
## Conformity assessment of test results

### Is the action or trigger value exceeded?



- Measurement uncertainty is taken into account in conformity assessment against thresholds such as action or trigger values.
- For the determination of measurement uncertainty, an approach is applied which may result in an asymmetrical interval under certain conditions

threshold is considered **not** to be **exceeded** when the entire measurement uncertainty interval of the test result lies below the action value



threshold is considered to be **exceeded** when the entire measurement uncertainty interval of the test result lies above the action value



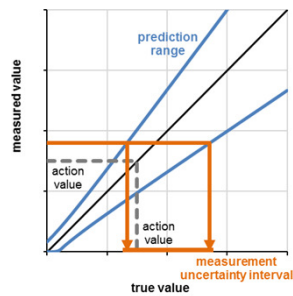
# Conformity assessment of test results

Is the action or trigger value exceeded?



- Measurement uncertainty is taken into account in conformity assessment against thresholds such as action or trigger values.
- For the determination of measurement uncertainty, an approach is applied which may result in an asymmetrical interval under certain conditions

No clear decision possible because the action value lies within the measurement uncertainty interval



- Recommendations are given as to how to reduce measurement uncertainty
- These recommendations are based on identifying the major sources of uncertainty; e.g. in the case of a large fundamental variability, finer grinding and/or increased sample volume

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de 9

# Webtool for calculating measurement uncertainty



- The concepts developed in the guidelines are implemented in a proprietary web service which is available at

<https://messunsicherheit-bbodschi.quodata.de/new/upload.html>

**Main menu**

- Home
- Software
- Interlaboratory Studies
- Seminars
- Research and Development
- Blog
- Web Services**
- 01: Internal webtool
- 02: External webtool
- 03: Data webtool
- 04: Soil prediction
- Seminars and Workshops
- Company

Web-services for analytical quality assurance

**In General**

Quodata has developed a variety of web applications in various projects, e.g. the [01: Internal webtool](#), a web application for [02: External webtool](#) and the [03: Data webtool](#). These enable the user to access certain services from any computer. Only an Internet connection and a browser are required for use.

Here you can find a selection of web applications developed by Quodata GmbH.

[01: Internal webtool](#)

[02: External webtool](#)

[03: Data webtool](#)

[04: Soil prediction](#)

Uncertainty | PCR Tool

**Web service for determination of uncertainty of results for assessment in accordance with Federal Soil Protection and Contaminated Sites Ordinance (Bundes-Bodenschutz- und Altlastenverordnung)**

The web application automatically determines whether the test result and its uncertainty is within the limit as set by the Federal Soil Protection and Contaminated Sites Ordinance (BodSchV) or whether the test result does not permit a clear evaluation. The results are provided in tabular and graphical form.

As part of its work for the German federal environment Agency's (UStA) Advisory Liaison on soil investigations, Quodata has developed the concept for the statistically-sound determination of the uncertainty of results on which the web application is based.

The evaluations of the web application can be used, among other things, for the preparation of expert opinions.

[Open application](#) [Request account](#)

Angemeldet als: **Hellner beaht**, noch 23:43 min. | [Abmelden](#) | [Kontrast ändern](#) | [neue Untersuchung](#) | [Übersicht](#) | [Beurteilen](#)

**Ermittlung der Ergebnisunsicherheit in BBodSchV**

**Dateneingabe**

004a\_BaP\_Wohngebiet\_ohne Vermahlen

**Situation**

Untersuchungspunkt  Orientierende Untersuchung  Detailuntersuchung

Wirkungspfad

Fächerschutz

Fächengröße

Mächtigkeit des Entnahmehorizonts

**Bodencharakteristika**

Bodenart

Kann die Homogenität der Schadstoffverteilung in der Fläche beurteilt werden?  Ja  Nein

Wie homogen verteilt sich die Schadstoffbelastung bzw. das belastete Porenvolumen in der Fläche? (100 % = homogen)

Wie groß ist der Durchmesser der kleinsten Fremdpartikel bzw. des kleinsten Porenvolumens im Durchschn.?

Welcher Anteil der Schadstoffbelastung stammt von Fremdpartikeln (also nicht von Bodenpartikeln)?

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de 10

## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

### Situation

Untersuchungsumfang:	Type of analysis:	<input checked="" type="radio"/> Orientierende Untersuchung	Exploratory investigation
		<input type="radio"/> Detailuntersuchung	Detailed investigation
Wirkungspfad:	Pathway	<input type="text" value="Boden - Mensch"/>	<input type="text" value="Soil - human"/>
Flächennutzung:	Use:	<input type="text" value="Wohngebiete"/>	<input type="text" value="Residential areas"/>
Flächengröße:	Size:	<input type="text" value="4000"/>	m <sup>2</sup>
Mächtigkeit des Entnahmebereichs:	Sampling depth:	<input type="text" value="10"/>	cm

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de  
11

## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

Coarse sand (up to 2 mm)  
Middle sand (up to 0.63 mm)  
Fine sand (up to 0.2 mm)  
Sand/Sluff (up to 0.063 mm)

### Bodencharakteristika

Bodenart:	Type of soil:	<input type="text" value="Grobsand (bis 2 mm)"/>
Kann die Homogenität der Schadstoffverteilung in der Fläche beurteilt werden?	<input checked="" type="radio"/> Ja	<input type="radio"/> Nein
	Can the distribution of contaminants in the site be assessed? ⓘ	
Wie homogen verteilt sich die Schadstoffbelastung bzw. das belastete Porenvolumen in der Fläche? (100 % = homogen)	<input type="text" value="100"/>	%
	Homogeneity of contamination in the site	
Wie groß ist der Durchmesser der belasteten Fremdpartikel bzw. des belasteten Porenvolumens im Durchschnitt?	<input type="text"/>	mm
	Size of contaminated non-soil particles ⓘ	
Welcher Anteil der Schadstoffbelastung stammt von Fremdpartikeln (also nicht von Bodenpartikeln)?	<input type="text"/>	%
	Proportion of contamination caused by non-soil particles	

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de  
12

## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

### Untersuchung von Einzel- oder Mischproben

### Analysis of single or mixed samples

Wurden Einzel- oder Mischproben analytisch untersucht?

Einzelproben

Mischproben

Anzahl Einzelproben je Mischprobe:

Number of single samples  
combined to a mixed sample

### Volumina und Vermahlungsgrad

Volumen der Laborprobe:

L

Lab sample volume



Wird die Laborprobe vermahlen?

Ja

Nein Has the sample been grinded?

Masse der Analysenportion:

g

Test portion mass

Webtool for taking measurement uncertainty into account in the implementation  
of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de  
13

## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

### Labor und Anzahl Bestimmungen

### Analysis in one or several labs?

Wurde(n) die Probe(n) in einem oder mehreren Laboratorien  
untersucht?

in einem Labor

in mehreren Laboratorien



Anzahl Mehrfachbestimmungen je Probe:

Number of replicates  
for each sample

### Angaben zur analytischen Methode

HorRat-Wert:



HorRat value: ratio of reproducibility s.d. and Horwitz s.d.

Webtool for taking measurement uncertainty into account in the implementation  
of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de  
14

- Example: Benzo(a)pyrene

**Messwerte**  Measured values

Analyt	Benzo(a)pyren	Benzo(a)pyren	
Prüfwert	Trigger value	4	
Maßnahmenwert	Action value	nicht in BBodSchV geregelt	
Einheit	Unit	mg/kg TM	
Mischprobe	Untersuchungsergebnis	Untersuchungsergebnis	test result
Mixed sample	1	3,9	5,5
	2	8,1	10,8
	3	4,3	3,6
	4	5,7	7,4
	5		

- Example: Benzo(a)pyrene

**Bewertungsergebnis** Assessment

Analyt:	Benzo(a)pyren
Prüfwert: trigger value	4.00 mg/kg TM
Maßnahmenwert: action value	nicht in BBodSchV geregelt mg/kg TM
Untersuchungsergebnis (Mittelwert aus 4 Mischprobe(n)):	test result 5.50 mg/kg TM
Ergebnisunsicherheitsbereich: measurement uncertainty range	3.94 - 8.05 mg/kg TM
Indizienkraft: evidence level	94 %
Analytische Unsicherheit inkl. Fundamentalvariabilität: Uncertainty of analysis method and fundamental variability	3.98 - 7.89 mg/kg TM

Die Untersuchung liefert keine eindeutige Bewertungsgrundlage.

Weitere Untersuchungen sind notwendig, um beurteilen zu können, ob ein Prüfwert überschritten oder unterschritten ist.

The investigation does not provide a clear basis for evaluation.  
Further examinations are necessary in order to assess whether a trigger value is exceeded or not.

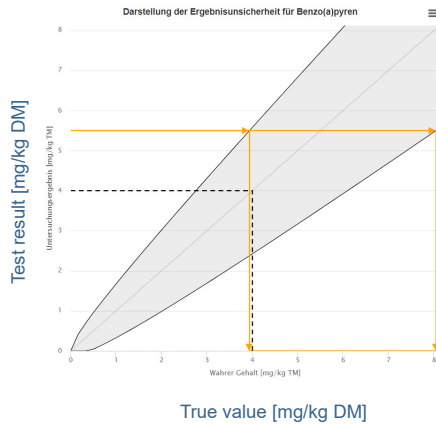


## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

coarse sand (up to 2 mm)



Major source of uncertainty: fundamental variability

### Recommendations:

The scope of the investigation should be extended in order to reduce the measurement uncertainty. Otherwise a detailed investigation should be considered. Alternatively, risk assessment may be performed on a case by case basis.

### Maßgeblich verantwortliche Unsicherheitskomponente(n):

- Fundamentalvariabilität der Analysenprobe

### Empfehlungen:

Es ist in Betracht zu ziehen, den Untersuchungsumfang zu erweitern, um die Ergebnisunsicherheit zu reduzieren. Andernfalls sollte eine Detailuntersuchung in Betracht gezogen werden. Alternativ kommt in Betracht, die Gefährdungsabschätzung gegebenenfalls auf Grundlage anderer Umstände des Einzelfalles abzuschließen.

Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

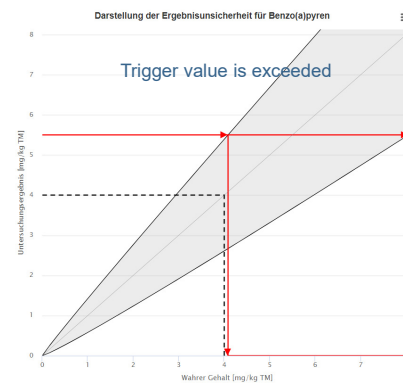
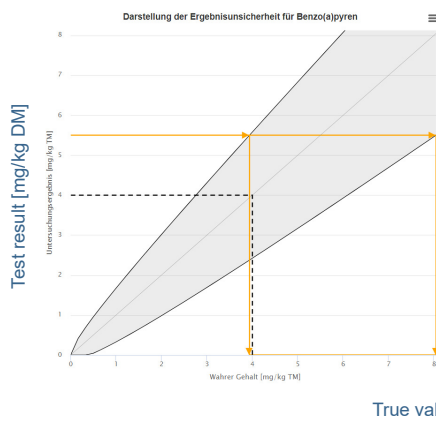
www.quodata.de  
17

## Webtool for calculating measurement uncertainty



- Example: Benzo(a)pyrene

coarse sand (up to 2.0 mm) → fine sand (up to 0.2 mm)



Webtool for taking measurement uncertainty into account in the implementation of the Federal Soil Protection and Contaminated Sites Ordinance

www.quodata.de  
18

## Webtool for calculating measurement uncertainty



- Within a research project, a concept has been developed for the determination and application of measurement uncertainty in the context of the implementation of the Federal Soil Protection and Contaminated Sites Ordinance.
- A web tool has been developed that automatically calculates the measurement uncertainty for soil analysis
  - Decision support, e.g. for authorities or experts
  - Planning tool for sample design
  - Showing major sources of uncertainty
- The webtool is flexible and can be customized for other applications.



Thank you for your attention!

QuoData GmbH  
10787 Berlin, Ansbacher Straße 11  
01309 Dresden, Prellerstraße 14  
E-Mail: hettwer@quodata.de