Explanations to the Web Map Service (WMS) „Groundwater background values of Germany (HGW)“

Working group 'Groundwater Background Values' (PK Hintergrundwerte Grundwasser[1]) of the Ad hoc Working Group Hydrogeology (Ad-hoc AG Hydrogeologie) of the Geological Surveys of the Federal States of Germany (SGD); Status of documentation 28.01.2020, status of data: 06.10.2014

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1. Introduction

One of the main objectives of the EC Water Framework Directive (EC-WFD, German: EG-Wasserrahmenrichtlinie: EG-WRRL) is to achieve a good qualitative status of groundwater bodies. Good knowledge about natural background concentrations is essential to assess the groundwater quality depending on the regional geological conditions. This information is required to identify and quantify significant contamination and to propose appropriate counter measures.

To fulfill the requirements of the EC-WFD, the State Geological Surveys of Germany formed a working group (WG EC-WFD) as a coordinating committee. A main product of the activities of the WG EC-WFD is the Hydrogeological Map of Germany 1:200 000 (HUEK200). In 2019 the HÜK200 was migrated to HÜK250 (https://www.bgr.bund.de/huek250).

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A subgroup of the WG EC-WFD, the working group 'Groundwater Background Values' (WG GBV; in German: Personenkreis Hintergrundwerte, PK HGW) has established criteria for defining groundwater background values – in the context of quantifying natural interactions between aquifer matrix and groundwater - since 2005. This included the development of a nation-wide standardized approach for the derivation of background values, based on spatial hydrogeochemical (HGC) units, for a set of major and trace elements. The spatial extent of the HGC units and their statistic properties were linked to the HUEK200.

The outcome of this project is publicly available as Web Map Service (WMS) at https://services.bgr.de/wms/grundwasser/hgw/?

Given the geometric basis, the application operates at the macro-scale and hence provides an overview at the national and regional scale. Therefore, for specific questions, the map cannot replace a detailed case-by-case analysis at the local scale. Nevertheless, the WMS may contribute to fulfil requirements of the EC-WFD by allowing the integration of groundwater analytical results in a regional context, ultimately indicating potential local contaminations. Furthermore, it enables the recognition of naturally induced regional violations of threshold values in case-by-case assessments: "If regional geogenic background values exceed the minor threshold value, authorities in charge […] will be able to establish target values for individual cases" (excerpt from LAWA 2004).

In the following, the methodology and workflow of the statistical analysis applied on the original data set for deriving the groundwater background values are explained. The content of the WMS is described and instructions for the user are provided. The appendix lists all HGC units of Germany.

Based on a nation-wide database on groundwater characteristics, an initial assessment was carried out and made available on the internet in March 2009 (WAGNER et al., 2011). As the initial data pool (from 2005) was incomplete regarding spatial coverage, additional data were collected for the most relevant trace elements with available minor threshold values (LAWA 2004: arsenic, boron, barium, cadmium, cobalt, chromium, copper, fluoride, mercury, molybdenum, nickel, lead, antimony, selenium, thallium, vanadium, zinc) and for uranium, which was newly added to the German drinking water guideline (TRINKWV) in 2012. The latest statistical analysis of these parameters significantly increased spatial coverage. However, there are still HGC units with unsatisfactory data coverage, not permitting for spatial evaluation and presentation.

The assessment resulting from the new data collection was released in 2014. The publication by WMS will enable future survey updates compliant with a new data situation.

2. Objective and approach

The physical and chemical properties of groundwater are mainly influenced by the composition of the seepage water, its alterations during passage through the unsaturated zone, the lithology of the aquifer, and its residence time in the subsurface. The natural geogenic properties of groundwater are the result of a dynamic equilibrium between the fluid and the rock surface, where complex chemical, physical, and biological processes take place. Old and therefore mainly deep groundwater is primarily influenced by geogenic processes, while younger and shallower waters tend to show more surface related impacts, including human influence. In such aquifers, the natural geogenic-controlled composition of groundwater can often no longer be assessed. Thus, the background values in these cases represent a combination of the geogenic base and an ubiquitous diffuse anthropogenic component (WAGNER et al., 2003, KUNKEL et al., 2004).

The main objective of the WG BGV was a nationwide compilation of groundwater background values on the basis of available groundwater analyses from all over Germany. The groundwater data were provided by the competent authorities of each federal state in 2005 (the initial assessment was based on ~ 52,000 samples) and 2012 (new assessment for anorganic parameters with available minor threshold values according to LAWA 2004, and uranium). Thus, the measurements originate from groundwater samples collected between 1980 and 2012. The latest and most comprehensive analysis from each sampling point was used for the evaluation.

Before the derivation of background values, groundwater samples with known anthropogenic contamination, e.g. from monitoring bores in the vicinity of landfills or contaminated sites, were discarded from the database. In particular, the groundwater samples from the city states Berlin, Hamburg and Bremen are to a great extent influenced by human activities. Also, these states have a denser groundwater monitoring network than the rest of Germany and thus the consideration of all samples would have led to a bias in the data set. Therefore, samples from these three states were excluded according to the criteria provided by the 'Berliner Liste' (SENSTADT, 2005). The threshold values of chloride and ammonium were not employed for Hamburg and Bremen as higher concentrations of these parameters are naturally occurring in the area. In addition, due to the strongly depth-dependent variations in groundwater quality in the aquifers of the North and Central German unconsolidated rock region (GR01), the data set for this region was restricted to groundwater samples of a depth < 50 m. After this pre-selection the nationwide data set of the 2005 collection used for determination of background values included ~ 45,000 samples. The 2012 data collection includes between 13,000 and 24,000 samples, depending on the trace element evaluated.

In preparation of the statistical evaluation, about 1,100 hydrogeological units of the current Hydrogeological Map of Germany 1:200 000 (HUEK200) were aggregated into HGC units based on geologic-genetical and lithological criteria. HGC units are defined as hydrogeological units with typical distributions of hydrogeochemical properties maintaining a compilation according to the ten hydrogeological regions. Depending on its geographic position and the aquifer at its sampling depth, each sample was then assigned to the appropriate HGC unit.

For the northern region (GR01), this approach led to very large units that could not represent the lateral and vertical hydrogeochemical inhomogeneities originating from different geogenic influences such as coastal and inland salinization, marshes or brown coal deposits. Therefore, the HGC units in this region had to be defined and delineated by a different approach. As the hydrogeological sub-regions show a much higher degree of differentiation in this area and since their definition is also based on hydrogeological criteria, these sub-regions were aggregated into geochemically similar HGC units and samples were assigned to the respective HGC unit based on their geographical position.

After each groundwater sample had been assigned to a HGC unit, the data were assigned to the ten hydrogeological regions (see Appendix) and statistical analyses were performed (Table 1). A total of 186 HGC units were defined, of which 112 units contained sufficient (i.e. 10 or more) samples to perform the statistical analysis. The evaluated units cover about 97.5% of Germany.

Table 1: Statistical evaluation of the HGC units within the hydrogeological regions

Hydrogeological Region (in German)	**Hydrogeological Region (English translation)**	**Token**	**Interpreting Geological Survey/State**	
			Data pool 2005	Data pool 2012 (trace elements)
Nord- und mitteldeutsches Lockergesteinsgebiet	North and central German unconsolidated rock region	GR01	BGR / Federal agency, LBEG / Lower Saxony	BGR / Federal agency, LfULG / Saxony
Rheinisch-Westfälisches Tiefland	Rhenish-Westphalian lowland	GR02	GD / North Rhine-Westphalia	GD / North Rhine-Westphalia
Oberrheingraben, Mainzer Becken und Hessische Senke	Upper Rhine Graben, Mainz basin and Hessian depression	GR03	BGR / Federal agency	HLUG / Hesse
Alpenvorland	Alpine lowland	GR04	BGR / Federal agency	LfU / Bavaria
Mitteldeutsches Bruchschollenland	Central German fault block region	GR05	TLUG / Thuringia	TLUG / Thuringia
West- und süddeutsches Schichtstufen- und Bruchschollenland	West and South German escarpment and fault block region	GR06	BGR / Federal agency	BGR / Federal agency
Alpen	The Alps	GR07	LfU / Bavaria	LfU / Bavaria
West- und mitteldeutsches Grundgebirge	West and Central German crystalline basement	GR08	LGB / Rhineland-Palatinate	LGB / Rhineland-Palatinate, BGR / Federal Agency
Südostdeutsches Grundgebirge	Southeast German crystalline basement	GR09	LfULG / Saxony	LfULG / Saxony
Südwestdeutsches Grundgebirge	Southwest German crystalline basement	GR10	BGR / Federal agency	BGR / Federal agency

The statistical evaluation of each parameter was performed semi-automatically using probability plots (Walter et al., 2012, see Section 3). This method allows the identification of distinct populations. Thus, anomalies can easily be identified and separated from the background population. These anomalies (Marczinek et al., 2008) could be caused by anthropogenic influences of diffuse or point sources, but also by natural phenomena such as coastal and inland salinization (Grube et al., 2000), or acidification of crystalline rock regions (Hinderer & Einsele, 1998). However, the application of this method is limited if the anthropogenic impact of long term atmospheric and agricultural inputs (e.g. fertilization, soil melioration, traffic related inputs) has reached a level which integrates as normal population into the full data set. Kunkel et al. (2004) established the term ‘natural, ubiquitously influenced groundwater composition’. For selected parameters (e.g. sulphate or chloride), the background populations show a ubiquitously elevated concentration profile (e.g. Upper Rhine Graben), which cannot be easily separated with the applied method. A specific entry in the info-query alludes to this phenomenon.

The statistical parameters (mean, standard deviation, percentiles) of the normal distribution can be derived from their position in the probability plot. The upper limit of the parameter specific background values is defined as the 90th percentile in a HGC unit, which is the concentration undercut by 90% of the measurements.

The statistical results were validated and, if necessary, modified by the geological surveys responsible for the respective HGC unit. The tables with the final results were then included into the HUEK200 database by BGR and transferred to the Web Map Service.

3. Method: Derivation of background values with probability plots

If the groundwater background values are defined as the natural regional groundwater composition, it might seem that under similar regional conditions groundwater should show a more or less uniform, normal or lognormal distribution of chemical parameters. In reality, though, the chemical composition of groundwater is the result of many chemical reactions and other natural and anthropogenic influences, which act on different temporal and spatial scales. The concentration distribution can be affected - with varying intensity for each parameter - by different initial concentrations, changes in the reaction mechanisms, varying transmission paths, or various external influences, e.g. vegetation, atmospheric, or anthropogenic ones. Anomalies and different subpopulations will affect the parameter distributions with a growing number of samples and increasing size of the investigated area. It is the aim of this project to decide if multiple peaks or breaks in the cumulative curve or histogram of a data set should be interpreted as the existence of subpopulations. The interpretation depends largely on the experience of the evaluator. Methods such as the probability net, which allow at first glance an evaluation of the distribution (normal or lognormal) and an easy distinction of separate populations, are thus of great advantage.

For decades exploration geochemistry has successfully used statistical methods to identify and delineate anomalies resulting from ore mineralizations, which are of natural and geogenic origin. In this context, an anomaly is defined as a deviation from the characteristic regional distribution and can be found in the higher as well as in the lower segments of the concentration range (VAN DEN BOOM, 1981). While in ore exploration the lower boundary of the anomaly is of interest for separating the high concentration of the anomaly from the less important lower concentration of the background, the upper boundary of the normal population is of interest for hydrogeological investigations. Despite this slightly different viewpoint the statistical methods used in exploration geology can be transferred to groundwater data in order to identify local and regional anomalies within the normal population.

LEPELTIER (1969) developed a method on the basis of probability plots using cumulative percentages, which is now an established standard in exploration geology. The method had to be slightly adjusted as the identification and calculation of distribution parameters for anomalies is somewhat different from the approach of determining groundwater background values, which are solely related to the normal population.

The probability plot is a simple graphical procedure to determine the distribution of a random variable. The graph shows the concentration on a linear x-axis over an integrated normal distribution on the y-axis:

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} \, \mathrm{d}t$$

Normal distributions or normally distributed sections of a random variable are thus represented by a straight line (Figure 1). This allows for a simple visual examination of the data set at hand and facilitates a quick distinction between normal and anomalous components. The great advantage of the probability plot is that the statistical distribution parameters of the different line sections can easily be determined: the median corresponds to the arithmetic mean of the population (i.e. cumulative sum of 50%) while the slope defines the standard deviation. Lognormal distributions also produce a straight line if the x-axis is scaled logarithmically.

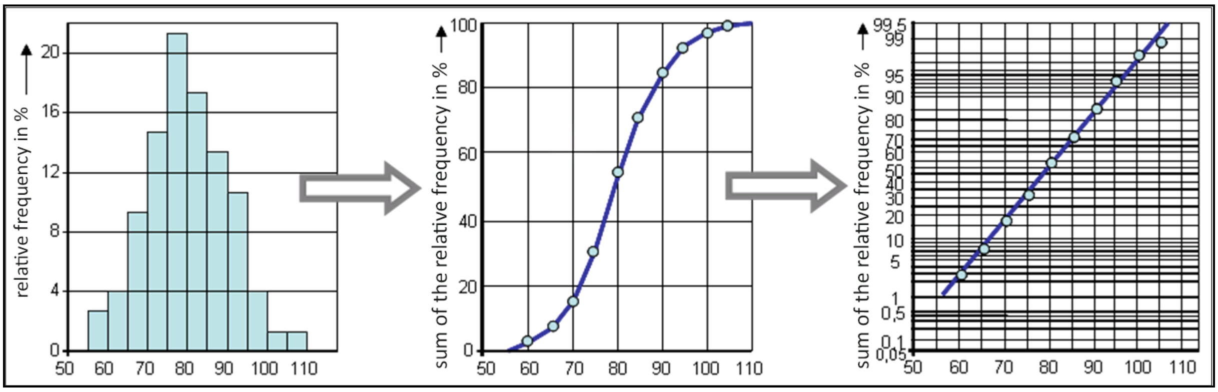


Figure1: Transformation from the histogram over the cumulative sum curve to the probability plot (after Din 53804-1).

Mixtures of populations appear as straight line segments with different slopes and lengths on the graph and thus can be distinguished easily. While each population has a characteristic straight section, there are also transition segments on each end of that section. The latter can be identified by their higher standard deviation, which is characteristic for mixed populations. Sinclair (1979) and Van den Boom (1981) describe the rationale for the most frequent combinations of straight lines in the probability plot. The probability plot thus allows an estimation of the heterogeneity of the data set at first glance. Therefore, it is advised to examine the complete data set before excluding data.

By means of the abovementioned procedure the line segment with a slope characteristic for the background population is selected. The corresponding distribution of values is then utilized for the calculation of mean, standard deviation, and the respective percentiles (Figure 2a). Commonly the 90th or 95th percentiles are being used to define the upper limit of background concentrations. For this project the groundwater background value was defined as the 90th percentile.

Values below the detection limit can also be accounted for by this procedure. For this purpose the percentage of values below the detection limit is added to the cumulative curve. This compresses the range of standard deviation of the measured data and moves it to the right, thus effectively extending the range of concentration values below the detection limit. The extrapolation of the line is valid as long as the whole population can be assumed to be homogenous. This is warranted as long as the assumption of a (log)normal distribution is not rejected below the detection limit due to bimodality or other indications that would result in a different distribution (Figure 3). It has to be noted, though, that the detected values of minor and trace elements with a high percentage of samples below the detection limit could represent an upper anomaly. This could only be verified if the detection limit for those parameters were lowered, so that enough measured data would be available.

For an efficient and descriptive evaluation, a software tool was developed in Microsoft Excel which iteratively visualises a trend line to the main population of the distribution, thereby excluding anomalies on both sides of the distribution (Figure 2a). In most cases the tool allows a quick user controllable semiautomatic adaption of the dataset to straight lines representing different populations separated by the inflection points of the curve. If large numbers of anomalous values exist, the procedure can be accelerated by removing those values after the initial examination of the data set.

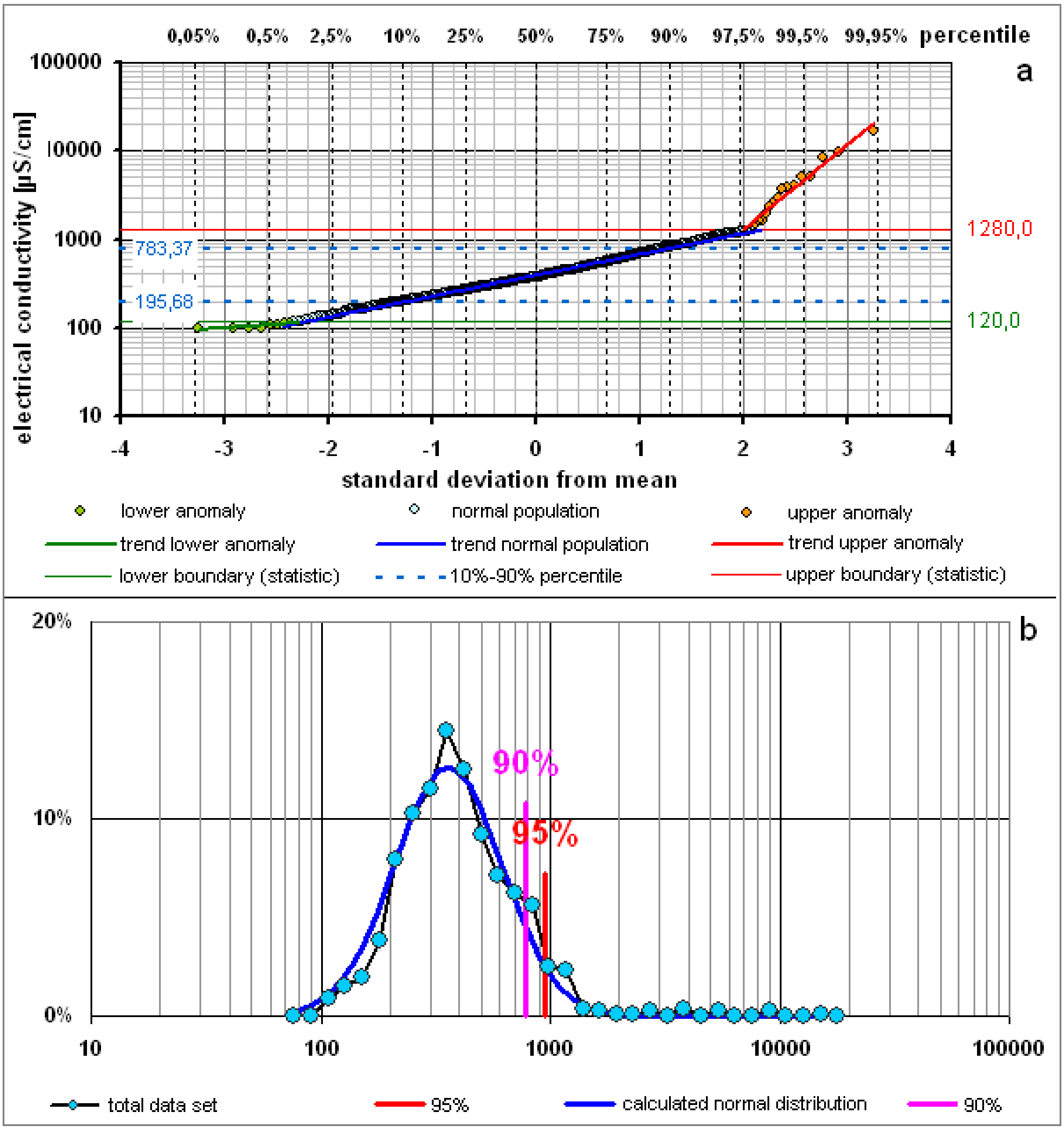


Figure 2: a: Distribution of the electrical conductivity EC (µS/cm) in the HGC unit 01R14c Brandenburger Jungpleistozän. The steep section of the upper anomaly can clearly be identified while the slope of the lower anomaly is not fundamentally different from that of the normal distribution. The values between 100 and 1280 µS/cm were included to calculate the background value (90th percentile) (see Table 2). Compared to Figure 1, the x- and y-axis are transposed, so the slope allows a direct judgement of the standard deviation (steep = high, gentle = small standard deviation).

b: Graphical representation of the total population as a histogram overlaid with the calculated normal distribution.

The results can be cross-checked visually by comparing the calculated normal populations to a histogram of the data (Figure 2b). Goodness of fit is also tested by the correlation coefficient and the d'Agostino-Pearson-test for normality (SHESKIN, 2007). These tests allow an easy verification of the concordance of assumed and actual distributions, i.e., whether the data are best represented by a normal or lognormal distribution. The final result is calculated after the temporary deletion of all anomalies and allowing no further exclusion of values by the Excel tool (Alpha = 0%) (see Table 2). In addition, the plausibility of the data is assessed in context of the regional hydrogeology.

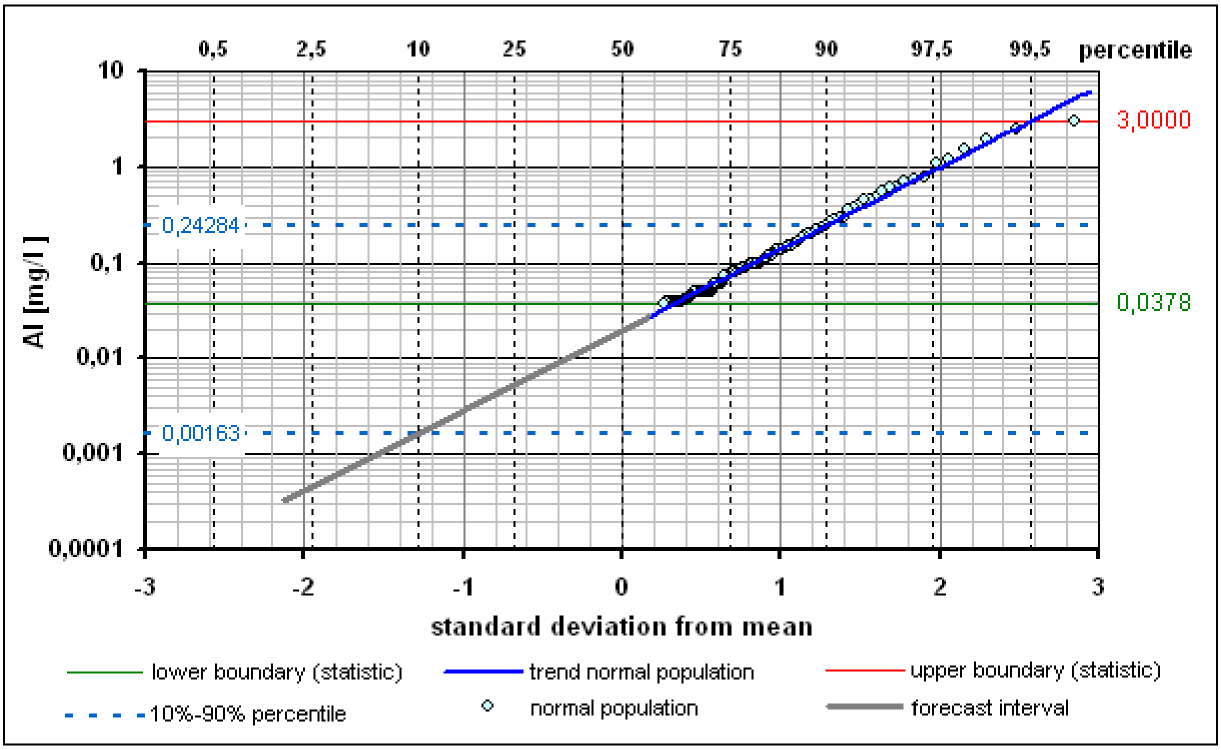
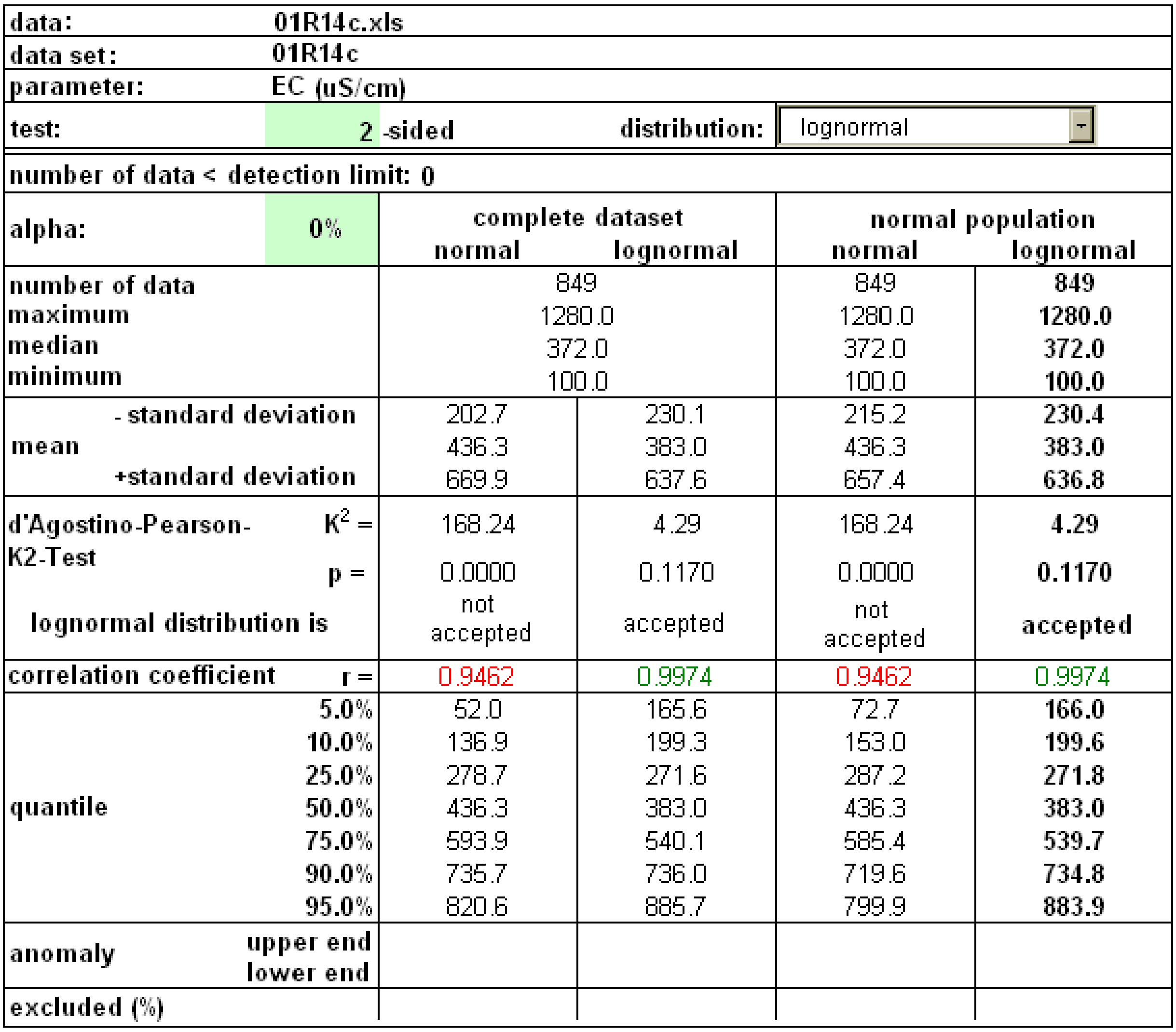


Figure 3: Data set with 60% of all values below the detection limit (aluminium (mg/l)) of the HGC unit 01R13b Mitteldeutsche Urstrom- und Nebentäler. By extending the line into the lower range, mean (intersection with 50% line) and standard deviation (slope) can be calculated. Hence, the percentiles below the detection limit can also be assigned.

A minimum of 10 measured values in the normal population (i.e. without data below detection limit and excluded anomalies) was defined to guarantee statistical reliability. In addition, over 60% of all data for major elements (see Table 3) had to be included in the normal population for a valid background value. This criterion was not adopted for minor and trace elements as it would have resulted in an exclusion of many results due to high percentages of data below the detection limit. If 90% of the measurements specific to a trace element are below the limit of analytical determination, the 90th percentile cannot be ascertained by the (discrete) values. In this case the spatial visualisation of the WMS shows the lowest value class, but without a discrete 90th percentile value in place. An explicative note will then be displayed in the info box.

The method for separating anomalies from the data set is in principle comparable to the method of KUNKEL et al. (2004), who separated anomalies based on the shape of the histograms. Probability plots have the advantage to be applicable even to smaller data sets and they allow an easier identification of populations on the basis of the inflection points in the probability net.

Table 2: Statistical metadata to the analysis presented in Figure 2, after exclusion of the upper 16 values (2.77% of all data). The lognormal distribution is accepted for the normal population (right column). Values below detection limit were not present. The correlation coefficient (r) is given and its significance is signalised by a colour coding (red = not significant, green = significant, bold green = highly significant)



data:	**01R14c.xls**				
data set:	**01R14c**				
parameter:	**EC (uS/cm)**				
test:	**2 -sided**		**distribution:**	lognormal	
number of data < detection limit: 0					
alpha:	**0%**	**complete dataset**		**normal population**	
		normal	**lognormal**	**normal**	**lognormal**
number of data		849		849	**849**
maximum		1280.0		1280.0	**1280.0**
median		372.0		372.0	**372.0**
minimum		100.0		100.0	**100.0**
	- standard deviation	202.7	230.1	215.2	**230.4**
mean		436.3	383.0	436.3	**383.0**
	+standard deviation	669.9	637.6	657.4	**636.8**
d'Agostino-Pearson-K2-Test	**K^2 =**	168.24	4.29	168.24	**4.29**
	p =	0.0000	0.1170	0.0000	**0.1170**
lognormal distribution is		not accepted	accepted	not accepted	**accepted**
correlation coefficient	**r =**	0.9462	0.9974	0.9462	0.9974
quantile	**5.0%**	52.0	165.6	72.7	**166.0**
	10.0%	136.9	199.3	153.0	**199.6**
	25.0%	278.7	271.6	287.2	**271.8**
	50.0%	436.3	383.0	436.3	**383.0**
	75.0%	593.9	540.1	585.4	**539.7**
	90.0%	735.7	736.0	719.6	**734.8**
	95.0%	820.6	885.7	799.9	**883.9**
anomaly	**upper end**				
	lower end				
excluded (%)					

4. Data presentation as Web Map Service

The results of the project ‘Groundwater Background Values’ are available to the public as a WMS (at the moment in German only, English version is in preparation). With this service the background values can be accessed as maps (Figure 4) and info-queries (Figure 5) can be launched. The results can be viewed with WMS-capable programs or via an internet application, e.g.:

- Google Earth, ESRI ArcGIS Explorer etc.,
- Geographic Information Systems (GIS),
- Internet map browsers with WMS import function.

The WMS can be accessed via the following internet addresses (URL with or without parameters):

- https://services.bgr.de/wms/grundwasser/hgw/?

- https://services.bgr.de/wms/grundwasser/hgw/?REQUEST=GetCapabilities&VERSION=1.3&SERVICE=WMS&

The URL address has to be added to the WMS capable program. Usually, the URL without parameters is sufficient. Otherwise the URL with parameters should be used. At https://geoviewer.bgr.de/ the WMS has already been integrated and can be viewed.

This way every user can access the background values, display maps and investigate the values in the database via info-queries.

5. Presented contents

Hydrogeochemical units

The information presented in the WMS is arranged in thematic layers and comprises the 10 hydrogeological regions (GR01 to GR10) of Germany. These regions are further subdivided into HGC units whose boundaries and ID numbers are available in extra layers. A HGC unit describes a hydrogeological unit with a characteristic composition of groundwater components of the uppermost aquifer. It has to be noted that heterogeneities may still exist within the units, for example due to small scale lithologic alterations, which cannot be depicted at the scale of the project. Heterogeneities can be recognized by a high standard deviation in the data set.

The ID numbers of the HGC units are composed of the number of the region, a letter characterizing the age/lithology/subregion and a serial number (for example 06M5 -> region 06, Mesozoic, unit 5). A graph and a table with all HGC units are provided in the appendix.

Spatial visualisation of the background values

The maps of groundwater background values can be displayed for the 50th and the 90th percentile of representative values for each HGC unit and parameter. The 50th percentile is the mean value and the 90th percentile the upper limit of all representative values describing the groundwater composition in a unit.

Table 3: Hydrochemical and physicochemical parameters displayed in the WMS

Major elements	Minor and trace elements			Physicochemical parameters
Calcium (Ca)	Silver (Ag)	Iron (Fe)	Silicate (SiO2)	Total hardness
Chloride (Cl)	Aluminium (Al)	Lithium (Li)	Tin (Sn)	Specific electrical conductivity (LF)
Hydrogen carbonate (HCO3)	Bismuth (Bi)	Manganese (Mn)	Strontium (Sr)	pH-value (pH)
Potassium (K)	Bromine (Br)	Ammonium (NH4)		
Magnesium (Mg)				
Sodium (Na)				
Sulphate (SO4)				
	Trace elements (2012 assessment)			
	Arsenic (As)	Copper (Cu)	Antimony (Sb)	
	Boron (B)	Fluoride (F)	Selenium (Se)	
	Barium (Ba)	Mercury (Hg)	Thallium (Tl)	
	Cadmium (Cd)	Molybdenum (Mo)	Uranium (U)	
	Cobalt (Co)	Nickel (Ni)	Vanadium (V)	
	Chromium (Cr)	Lead (Pb)	Zinc (Zn)	

The procedure to identify the background values is explained in detail in section 3. In total 39 parameters (Table 3) were assessed. The data newly obtained and analysed in 2012 are presented separately. Not all HGC units could be evaluated for all parameters since the data coverage varies. Especially for numerous trace elements from several smaller HGC units sufficient data did not exist to fulfil the statistical minimum requirement (10 values in normal population). The data situation improved significantly by the new measurement collection of trace elements with available minor threshold values in 2012. The base values of these parameters were newly calculated as spatially-weighted mean values of the 90th percentile of the HGC units according to the procedure described in LAWA (2004) (Table 4).

No calculations were performed for nitrate, because nearly all elevated concentrations (~> 10 mg/l) are caused by anthropogenic impacts and thus they do not fit this topic.

Table 4: Parameter with minor threshold values according to the data collection and 2012 assessment: Total number, measurement locations, percentage of spatial coverage of assessed HGC units and spatially-weighted mean values of 90th percentiles in relation to the total area of Germany

Parameter	Total number sample locations	Spatial coverage in %	Base value (spatially-weighted mean values of 90th percentiles) [µg/l]
Antimony	14192	72%	0.17
Arsenic	24136	97%	3.21
Barium	16456	97%	175
Lead	24082	93%	1.05
Boron	22194	96%	116
Cadmium	24272	87%	0.3
Chromium	24067	94%	1.75
Fluoride	16014	89%	269
Cobalt	15073	82%	1.999
Copper	20747	96%	5.44
Molybdenum	13538	84%	1.34
Nickel	23109	78%	7.14
Mercury	13298	53%	0.088
Selenium	15810	80%	1.26
Thallium	13944	71%	0.0626
Uranium	15606	87%	3.45
Vanadium	14830	88%	1.68
Zinc	21077	96%	57.6

The statistically derived background values are divided into 6 colour coded classes, which are displayed within the areal extent of each HGC unit. Although in general the area of surface outcrop is used to map the respective HGC unit, special cases have to be considered. Following the three-dimensional geological structure the surface outcrop of a HGC unit is not necessarily congruent with its complete subsurface extent in a horizontal projection. Therefore, sample points related to a HGC unit, which is the main aquifer for water supply, may superficially be located outside of the mapped surface outcrop (see point data further down). Furthermore, there is no reproduction of three-dimensional variations of the parameter characteristics, which may appear either horizontally by area or vertically by depth. For instance, highly variable redox conditions referring to the spatially extensive HGC unit quaternary Upper Rhine Valley results in "distortions" as the reducing conditions in the northern part affect the percentiles of the Fe and Mn concentrations in the entire unit.

For groundwater background values the 90th percentile is of the highest interest, but in principle it is also possible to display other percentiles. After the revision in 2014 the WMS also includes 50th percentiles. Figure 4 shows the background value map for the example of 90th percentiles of arsenic. The lower boundary of the highest class of the six colour coded classes is usually based on a reference value[2] for each parameter. If no reference value exists, as in the case of hydrogen carbonate, the 90th percentile of all calculated background values from all HGC units (without weighing) is used instead. More than 75% of all HGC units exceed the reference value for the parameters iron (Fe) and manganese (Mn).

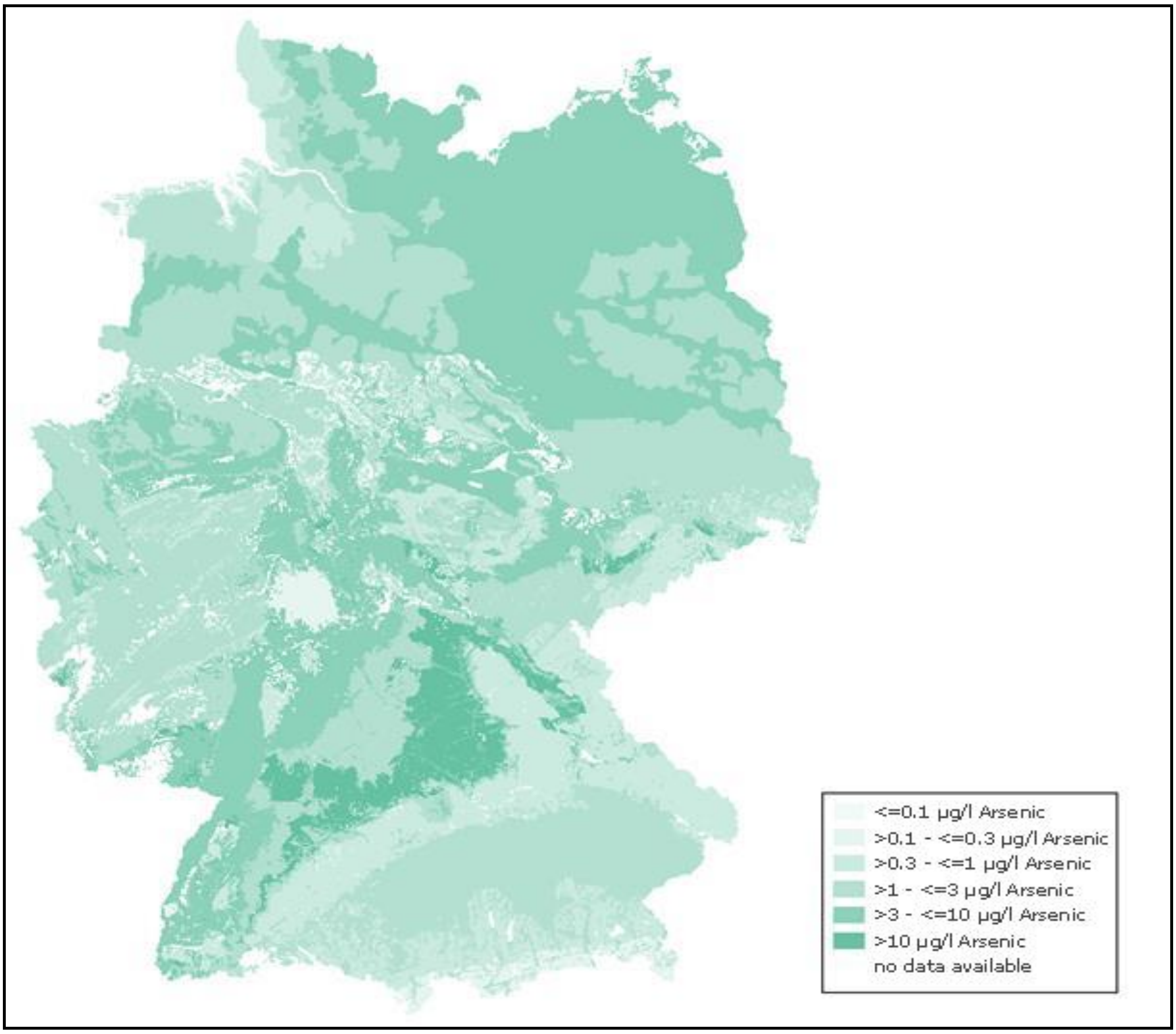


Figure 4: Map of groundwater background values (90th percentiles) for the example of arsenic

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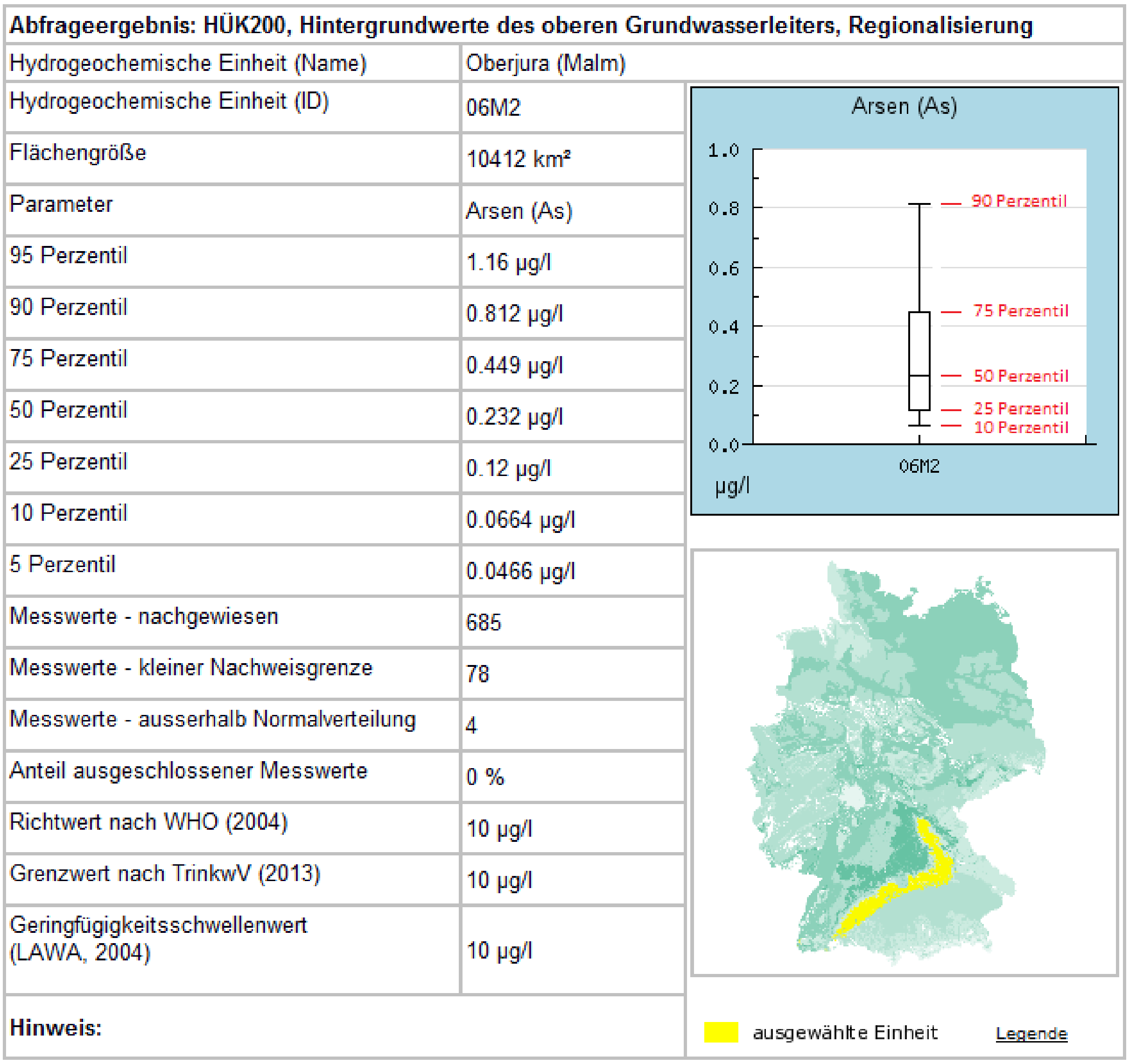
[2] The reference value is derived from threshold values and guidelines after Lawa (2004), TrinkwV (2013) and Who (2004).

Because these thresholds from the German drinking water guideline (TRINKWV) are only of aesthetic character, the highest class was established clearly above the corresponding reference value (10 respectively 1 mg/l) for a more meaningful map. Similarly, the highest class of ammonium was raised to 4 mg/l to achieve a more informative presentation as about 40% of all background values for ammonium (NH_4) are above the reference value of 0.5 mg/l due to geogenic influences. Units that had too little or no data for a parameter to be evaluated are displayed as legend class "no data available" in white color, respectively.



Abfrageergebnis: HÜK200, Hintergrundwerte des oberen Grundwasserleiters, Regionalisierung

Hydrogeochemische Einheit (Name)	Oberjura (Malm)
Hydrogeochemische Einheit (ID)	06M2
Flächengröße	10412 km²
Parameter	Arsen (As)
95 Perzentil	1.16 µg/l
90 Perzentil	0.812 µg/l
75 Perzentil	0.449 µg/l
50 Perzentil	0.232 µg/l
25 Perzentil	0.12 µg/l
10 Perzentil	0.0664 µg/l
5 Perzentil	0.0466 µg/l
Messwerte - nachgewiesen	685
Messwerte - kleiner Nachweisgrenze	78
Messwerte - ausserhalb Normalverteilung	4
Anteil ausgeschlossener Messwerte	0 %
Richtwert nach WHO (2004)	10 µg/l
Grenzwert nach TrinkwV (2013)	10 µg/l
Geringfügigkeitsschwellenwert (LAWA, 2004)	10 µg/l
Hinweis:	

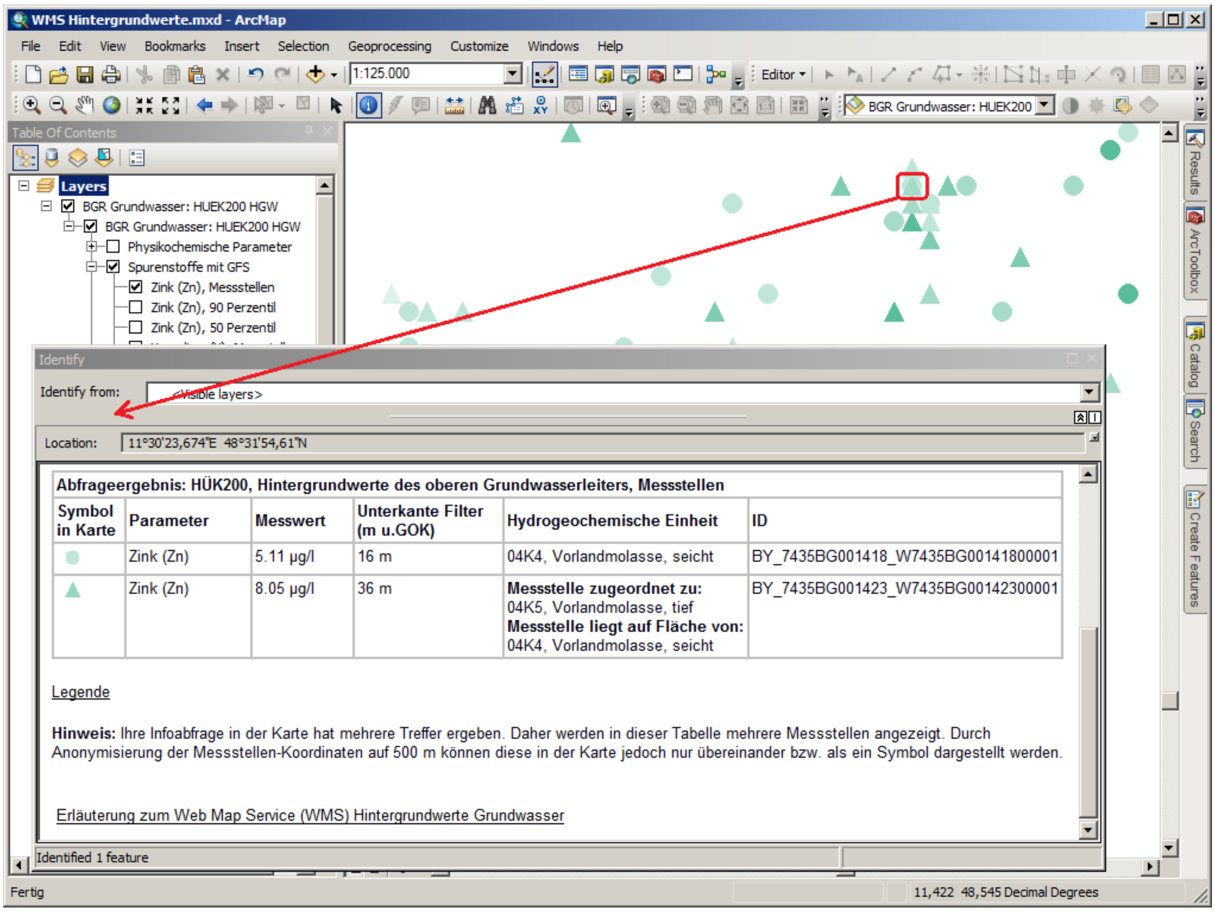
Figure 5: Result of an info-query for the example of arsenic in the hydrogeochemical unit 06M2 Upper Jurassic (Malm) in the hydrogeological region 6 (West and South German escarpment and fault block region).

Exceptions are units, in which less than 10 measurements are above the detection level and hence a normal distribution and theoretical indication of percentiles are not feasible. For these ranges without calculated distributions, the units are mapped in the lowest class of background values and the 90th percentile was specified as „< detection level". A query of the statistical analysis cannot present a distribution function and a note states: "The 90th percentile is in a range below detection level. It is not possible to perform a statistical evaluation of the distribution of background values" (see chapter 3).

Data retrieval via info-query

Apart from spatial information in the form of maps, further information about a HGC unit can be accessed via info-queries. This function can be used by clicking on the surface of the HGC unit in question. A new window opens with a table providing additional information on the selected HGC unit and parameter (in German only) (Figure 5). The info-query shows the areal extent of the selected unit in yellow (bottom right). Furthermore, name, ID and area of the selected HGC unit, as well as percentiles representing the geogenic distribution of values for the selected parameter are displayed. The percentiles are illustrated by a box plot (top right). The number 'data – detected' (Messwerte - nachgewiesen) comprises all values above the detection limit in the normal population, 'data – outside of normal distribution' (Messwerte - ausserhalb Normalverteilung) shows the number of values excluded from the evaluation. In addition, available reference values from WHO (2004), TRINKWV (2013) and LAWA (2004) are presented.

Apart from HGC unit specific background values, the actual data points are presented to document the database of the background values. The colour of the data points correlates with the colour codes of the background value classes. Hence a combination of polygon and point data gives an impression of the homogeneity/heterogeneity and regional variations of a specific parameter in a HGC unit. Data points can be selected as a separate layer in the WMS (Figure 6).



1:125.000

Layers
- ☑ BGR Grundwasser: HUEK200 HGW
  - ☑ BGR Grundwasser: HUEK200 HGW
    - ☐ Physikochemische Parameter
    - ☑ Spurenstoffe mit GFS
      - ☑ Zink (Zn), Messstellen
      - ☐ Zink (Zn), 90 Perzentil
      - ☐ Zink (Zn), 50 Perzentil

Identify from: <Visible layers>

Location: 11°30'23,674"E 48°31'54,61"N

Abfrageergebnis: HÜK200, Hintergrundwerte des oberen Grundwasserleiters, Messstellen

Symbol in Karte	Parameter	Messwert	Unterkante Filter (m u.GOK)	Hydrogeochemische Einheit	ID
●	Zink (Zn)	5.11 µg/l	16 m	04K4, Vorlandmolasse, seicht	BY_7435BG001418_W7435BG00141800001
▲	Zink (Zn)	8.05 µg/l	36 m	**Messstelle zugeordnet zu:** 04K5, Vorlandmolasse, tief **Messstelle liegt auf Fläche von:** 04K4, Vorlandmolasse, seicht	BY_7435BG001423_W7435BG00142300001

Legende

Hinweis: Ihre Infoabfrage in der Karte hat mehrere Treffer ergeben. Daher werden in dieser Tabelle mehrere Messstellen angezeigt. Durch Anonymisierung der Messstellen-Koordinaten auf 500 m können diese in der Karte jedoch nur übereinander bzw. als ein Symbol dargestellt werden.

Erläuterung zum Web Map Service (WMS) Hintergrundwerte Grundwasser

Figure 6: Info-query on data points for the example of zinc. The selected site contains two data points: a shallow bore in the upper aquifer corresponding with the surface HGC unit (circle symbol) and a deeper bore in a deeper aquifer corresponding to a different HGC unit (triangle symbol).

The application presents the single value used for the analysis, respectively. The point data is displayed nationwide in six colour classes (light to dark green) according to the classification of mapped areas. Due to data protection laws the location of the data points is arbitrarily shifted within a radius of 500 m, so they cannot be assigned to a specific borehole (inexact location).

The well screen of a given piezometer in a multi-aquifer formation is frequently located in a different (mostly deeper) HGC unit than the one that outcrops at the surface and is hence shown on the map. Those data points are displayed as triangles instead of circles. Again, an info-query for the point data provides further information on the selected bore (name and ID of HGC unit, measured value of chosen parameter, depth of well screen) (Figure 6).

Visualization of point data enables the user to evaluate local differences in data coverage and to compare the actual values in a certain area to the background value determined for the respective HGC unit. Regional anomalies can also be assessed because data points that were excluded from the normal population are displayed as well (except for preselected data).

6. Conclusions and outlook

The first spatially inclusive and comprehensive analysis of groundwater quality in West German aquifers was conducted by SCHLEYER & KERNDORFF (1992) with a relatively small data set of altogether 186 locations. KUNKEL et al. (2004) evaluated groundwater background values in Germany for major and trace elements from 40,000 groundwater samples differentiated into 17 hydrogeological units. The present investigation is based on about 45,000 groundwater samples (without update for trace elements) aggregated on the basis of hydrogeological units from the Hydrogeological Map of Germany (HUEK200) and the respective hydrogeological subregions, allowing for a more detailed differentiation (186 hydrogeochemical units). The results have been integrated into the HUEK200 database and in this way can be visualized as a WMS using the outcropping spatial extent of the uppermost aquifer for each HGC unit. In general, the results of the various investigations are similar, but increasing spatial resolution provides a more differentiated picture of local conditions. A possibly even higher resolution could be achieved by a catchment-based approach integrating the hydrogeological units of the more detailed hydrogeological map 1:50 000 (HK50).

The application is essentially updatable. Based on new measurements of trace elements hitherto not analysed yet, an initial update has already been implemented, focussing on administratively relevant trace elements with available minor threshold values (LAWA 2004). The most recent survey included between ~ 13,000 and ~ 24,000 sample locations, depending on the element evaluated. Additional assessments integrating new data or new legal requirements (e.g. for inventories) may be envisaged.

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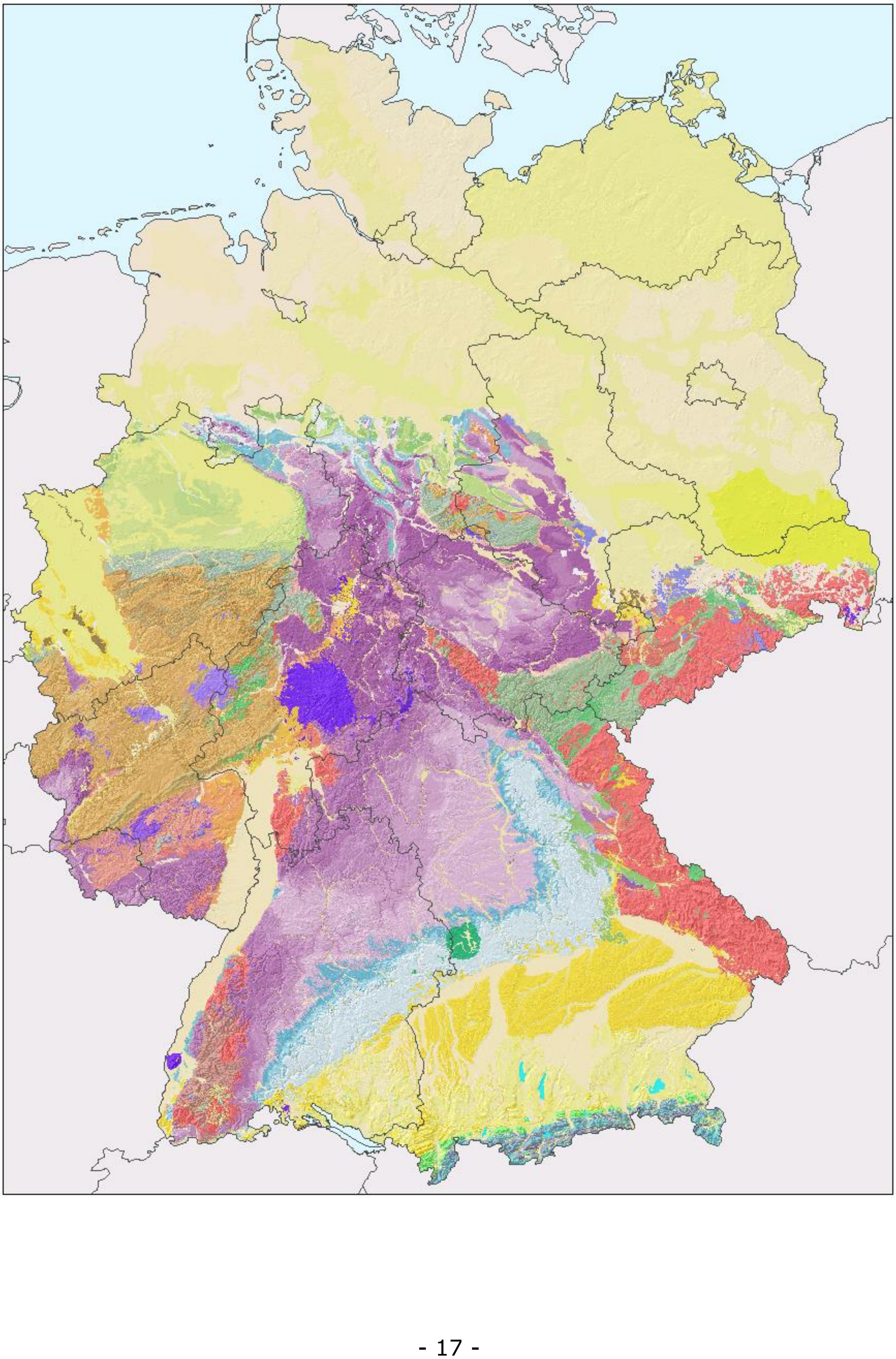
Appendix

Appendix 1: Map of the hydrogeochemical units.



Appendix 2: List of all HGC units for Germany sorted by region including area, number of evaluated parameters and number of aggregated HUEK200 units.

Note: The ID number of the HGC units comprise the number of the region (01-10), a letter characterizing the age/lithology/sub-region (K: Cenozoic, M: Mesozoic, P: Palaeozoic, V: vulcanite, R: sub-region) and a serial number increasing from stratigraphically younger to older units. The HGC units in region 01 comprise the number of the associated hydrogeological sub-region (R) and a further subdivision by a series of lower case letters for R13-R15.

Since the HGC unit names are fairly specific, a translation has not been attempted. Some general translations are: Jung = young, Mittel = middle, Alt = old, Niederung = lowland, Geest = moraine derived sandy region, Schluff = silt, Ton = clay, Kies = gravel, Kalk = limestone, Braunkohle = brown coal, silikatisch = siliceous, karbonatisch = containing carbonate, sulfatisch = containing sulphate, ungegliedert = unstructured

ID HGC	Name of hydrogeochemical unit (HGC)	Area [km²]	Number of parameters (max. 39)	Number of HUEK200 units
01R11	Nordseeinseln und Watten	4103,8	31	*
01R12	Marschen	6577,6	36	*
01R13a	Brandenburgische Urstrom- und Nebentäler	7830,3	22	*
01R13b	Mitteldeutsche Urstrom- und Nebentäler	7913,2	34	*
01R13c	Nordwestdeutsche Flussniederungen	4160,2	31	*
01R13d	Nordwestdeutsche Moorniederungen	4518,1	32	*
01R13e	Oberelbe-Mulde-Niederung	2806,8	31	*
01R14a	Schleswig-Holsteinisches Jungpleistozän	6676,4	29	*
01R14b	Mecklenburg-Vorpommersches Jungpleistozän	22841,0	29	*
01R14c	Brandenburger Jungpleistozän	11636,5	24	*
01R15a	Oldenburgisch-Ostfriesische Geest	2398,2	30	*
01R15b	Bederkesa-Zevener Geest	3643,2	31	*
01R15c	Nordwestdeutsche Geest	16225,0	33	*
01R15d	Nordost- und Mitteldeutsches Mittelpleistozän	13126,6	30	*
01R15e	Mitteldeutsches Mittelpleistozän	3630,4	35	*
01R16	Altmoränengeest	4097,0	30	*
01R17	Lausitzer Känozoikum	5768,0	31	*
02K1.2	quartäre Schluffe (Löss)	48,5		3
02K1.3	quartäre Sande, Kiese, Schluffe und Tone	10633,6	33	23
02K2.1	tertiäre Feinsande, Tone und Schluffe (ohne Brk.), östlicher Niederrhein	430,5	17	6
02K2.2	Braunkohlentertiär	66,0		6
02K2.3	tertiäre Sande, Schluffe und Tone (ohne Brk.), restlicher Niederrhein	959,1	22	27
02K3	Quellkalk	1,4		1
02M1	Unterkreide, silikatisch	321,2	11	14
02M10	Muschelkalk, karbonatisch-klastisch	4,4		4
02M11	Mittlerer Muschelkalk, salinar	0,1		1
02M12	Buntsandstein, tonig-salinar	0,9		2
02M2	Unterkreide, silikatisch-karbonatisch	130,3	11	8

ID HGC	Name of hydrogeochemical unit (HGC)	Area [km²]	Number of parameters (max. 39)	Number of HUEK200 units
02M3	Oberkreide, silikatisch	483,4	21	3
02M4	Oberkreide, silikatisch-karbonatisch	4533,1	31	26
02M5	Oberkreide, karbonatisch	952,8	20	9
02M6	Jura, ungegliedert	0,3		1
02M7	Malm, vorwiegend sulfatisch	4,9		1
02M8	Dogger	1,3		1
02M9	Lias	0,0		1
03K1	quartäre Kiese und Sande, silikatisch	273,2	3	3
03K2	quartäre Kiese und Sande, silikatisch-karbonatisch	6406,4	35	7
03K3	quartäre Sande und Schluffe, silikatisch	75,0		2
03K4	quartäre Sande und Schluffe, Quellkalke, karbonatisch	58,2		2
03K5	Tertiäre Grabenfüllung (Sande, Kiese, Schluffe)	508,9	18	3
03K6	Mio-Pliozän, limnisch-fluviatil (Mergel-, Ton-, Schluffstein)	926,6	22	5
03K7	tertiäre Karbonate (Kalktertiär)	640,9	18	1
03K8	tertiäre Tone und Mergel (Mergeltertiär)	916,4	15	6
03M1	mesozoische klastische und karbonatische Festgesteine	141,0		3
03V1	tertiäre Vulkanite	2566,5	21	3
04K1.1	quartäre Sande und Schluffe	0,1	17	4
04K1.2	quartäre Karbonate	23,1		1
04K2.1	quartäre Kiese und Sande, vorwiegend karbonatisch	12413,0	38	14
04K2.2	quartäre Kiese und Sande, vorwiegend silikatisch-karbonatisch	671,4	32	2
04K2.3	quartäre Kiese und Sande, vorwiegend silikatisch	66,0		2
04K3	quartäre Becken- und Moränenablagerungen	8923,0	36	9
04K4	Vorlandmolasse, seicht	12311,4	37	18
04K5	Vorlandmolasse, tief	0,0	20	
04V1	känozoische Vulkanite	25,8		1
05K1.2	quartäre Sande und Schluffe	1371,2	27	4
05K1.3	quartäre Kiese und Sande, silikatisch	3155,6	28	11
05K1.5	quartäre Karbonate (Travertin, Kalktuff)	52,5	1	4
05K2.1	Braunkohlentertiär	422,8	25	9
05K2.2	tertiäre Sande und Tone	188,8	25	8
05M3.1	Kreide silikatisch-karbonatisch	850,5	15	9
05M3.2	Kreide, vorwiegend silikatisch	1374,4	17	13
05M3.3	Kreide, vorwiegend karbonatisch	464,3	15	11
05M4.1	Jura undifferenziert	67,0		2
05M4.2	Malm, vorwiegend silikatisch-karbonatisch	519,5	18	8
05M4.3	Malm, vorwiegend sulfatisch	94,1		1
05M4.4	Dogger	420,1	15	7
05M4.5	Lias	1302,2	16	2

ID HGC	Name of hydrogeochemical unit (HGC)	Area [km²]	Number of parameters (max. 39)	Number of HUEK200 units
05M5.1	Trias	64,6		3
05M5.2	Keuper, klastisch	4822,3	27	11
05M5.3	Keuper, sulfatisch	1088,4	22	4
05M5.4	Muschelkalk, karbonatisch-klastisch	6104,4	31	8
05M5.5	Mittlerer Muschelkalk, salinar	349,0	16	1
05M5.6	Buntsandstein	12407,1	30	8
05M5.7	Buntsandstein, tonig-salinar	2078,5	20	3
05M6.1	Zechstein, ungegliedert (chloridisch, karbonatisch, sulfatisch)	1172,5	27	5
05M6.3	Zechstein, sulfatisch	162,5		4
05M6.4	Zechstein, klastisch	0,2		1
05M6.5	klastische Sedimente des Rotliegend	199,7	14	3
05M7	Mesozoikum (ungegliedert)	98,1		1
05P7.1	karbonische Ton- bis Sandsteine (aus GR 8)	44,4	11	4
05V2.3	tertiäre Vulkanite	229,0		10
06K1.1	quartäre Sande und Schluffe	37,7	30	2
06K2.1	quartäre Kiese und Sande, vorwiegend karbonatisch	231,4	10	4
06K2.2	quartäre Kiese und Sande, vorwiegend silikatisch-karbonatisch	908,6	28	3
06K2.3	quartäre Kiese und Sande, vorwiegend silikatisch	1509,9	35	4
06K3	tertiäre bis quartäre Sande und Kiese	72,7	13	4
06K4	Braunkohlentertiär	539,2	29	2
06K5	Ries-Trümmermassen	483,7	36	3
06K6	Bohnerz-Formation	17,4		1
06M1	Kreide	1030,9	35	4
06M10	unterer Muschelkalk, karbonatisch-klastisch	443,3	13	1
06M11	Buntsandstein, ungegliedert	10291,9	38	15
06M12	oberer Buntsandstein klastisch	827,2	10	1
06M13	Buntsandstein salinar	191,8	6	1
06M14	Trias ungegliedert	74,9	2	1
06M15	Perm, klastisch	776,8	34	8
06M2	Oberjura (Malm)	10461,6	39	12
06M3	Mitteljura (Dogger)	2442,8	38	5
06M4	Unterjura (Lias)	2484,7	35	6
06M5	mittlerer und oberer Keuper, klastisch	13387,5	37	21
06M6	mittlerer Keuper, salinar	368,6	37	4
06M7	unterer Keuper	4516,8	38	5
06M8	mittlerer Muschelkalk, salinar	997,7	33	3
06M9	Muschelkalk ungegliedert, karbonatisch-klastisch	6015,9	38	15
06P1	Metamorphite/Magmatite, sauer	0,7		2
06P2	Paläozoikum	0,5		1
06V1	tertiäre Vulkanite	24,3		3
06V2	Rotliegend-Vulkanite	56,3		1

ID HGC	Name of hydrogeochemical unit (HGC)	Area [km²]	Number of parameters (max. 39)	Number of HUEK200 units
07K1	Faltenmolasse	449,3	31	3
07M1	Helvetikum, Flysch	548,0	31	14
07M2	Kalkalpen, kalkig	1277,4	37	15
07M3	Kalkalpen, dolomitisch	1063,7	38	2
07M4	Kalkalpen, salinar	121,1	36	3
07M5	Alpiner Buntsandstein	6,2		1
07M6	Aroser Zone, Ultrahelvetikum und Feuerstätter Decke	52,6		1
08K1	quartäre Sande und Schluffe, silikatisch	120,0		1
08K2.1	quartäre Klastite	255,4	12	2
08K2.2	quartäre Klastite karbonatisch	2,6		1
08K3.1	quartäre Sande und Kiese	615,1	32	5
08K3.2	quartäre Sande und Kiese, karbonatisch	156,9		2
08K5	tertiäre Tone und Mergel (Mergeltertiär)	37,5		5
08K6	Mio-Pliozän, limnisch-fluviatil	4,0		2
08K7.1	tertiäre Sedimente	54,9		6
08K7.2	tertiäre Sedimente, silikatisch-organisch	15,8		3
08K8	tertiäre Tone	134,4		6
08M1	Oberkreide, karbonatisch	17,0		1
08M2	Oberkreide, silikatisch	45,9		3
08M3	Buntsandstein	223,8		2
08P1	Zechstein, vorwiegend sulfatisch/halitisch	98,4		3
08P10	paläozoische Karbonate	680,1	38	14
08P11	paläozoische Schiefer und Sandsteine	15847,5	30	25
08P12	paläozoische Schiefer, karbonatisch	2147,0	37	7
08P13	paläozoische Sandsteine und Quarzite	2093,2	42	7
08P14	paläozoische saure Ganggesteine	49,6		1
08P15	paläozoische saure Magmatite	180,0		2
08P16	paläozoische basische Magmatite	22,6		1
08P17	paläozoische Metamorphite	278,9		5
08P18	saure Plutonite	0,2		1
08P2	Rotliegend Klastite	3161,5	14	8
08P3	Rotliegend Sandsteine und Konglomerate	16,7		4
08P4	karbonische Sandsteine und Quarzite	193,1		3
08P5	karbonische Ton- bis Sandsteine	3886,7	44	12
08P6	karbonische Schiefer, karbonatisch	201,8		1
08P7	karbonische Karbonate	66,3		5
08P8	Ganggesteine des Karbon	2,6		1
08P9	karbonatische Schiefer	3,1		1
08V1	känozoische Basalte und Tuffe	1104,2	38	13
08V2	Rotliegend Vulkanite, sauer bis intermediär	253,2		3
08V3	Rotliegend Vulkanite, basisch bis intermediär	586,1		4
08V4	Vulkanite und Sedimentite des Rotliegend	22,9		2
08V5	paläozoische saure Vulkanite	108,5		2
08V6	paläozoische basische Vulkanite	55,3		2

ID HGC	Name of hydrogeochemical unit (HGC)	Area [km²]	Number of parameters (max. 39)	Number of HUEK200 units
08V7	saure Vulkanite	0,5		2
08V8	Metavulkanite	608,1	27	4
09K6.2	alttertiäre Kiese, Sande und Schluffe	135,0	8	2
09K6.3	Braunkohlentertiär Mitteldeutschland	105,7		6
09K6.4	jungtertiäre Kiese und Sande	13,7		2
09K6.5	Braunkohlentertiär Lausitz	30,1		1
09K7.1	quartäre Kiese und Sande, silikatisch	2215,6	29	25
09K7.2	quartäre Sande und Schluffe	369,9	28	1
09M2.1	Molasse, sedimentär (Oberkarbon und Rotliegend)	1010,9	28	9
09M3.1	Zechstein, karbonatisch	12,0	12	1
09M4.1	Buntsandstein, ungegliedert	5,8	28	2
09M5.1	Kreide, vorwiegend karbonatisch	284,7	28	9
09M5.2	Kreide, vorwiegend silikatisch	229,1	23	6
09P1.1	Paläozoikum ohne Perm schwach metamorph (Phyllite, Grauwacken, Tonschiefer)	5468,1	32	61
09P1.2	Metamorphite, karbonatisch	26,6	29	3
09P1.3	Metamorphite/Magmatite, sauer (Gneis, Glimmerschiefer, Granulit, Quarzit, Granit)	13894,8	37	72
09P1.4	Metamorphite/Magmatite, basisch (Metabasite, Diabas, Gabbro, Monzonit)	1317,6	34	28
09V2.2	Molasse, effusiv (Oberkarbon und Rotliegend)	801,9	27	30
09V6.1	tertiäre Vulkanite	99,9		5
10K1.1	quartäre Sande und Schluffe, karbonatisch	1,2		1
10K1.2	quartäre Sande, silikatisch	120,9		1
10K1.3	quartäre Kiese und Sande, silikatisch	5,6		1
10K1.4	quartäre Kiese und Sande, karbonatisch	40,8		1
10P1.1	basische und ultrabasische Silikatgesteine des kristallinen Grundgebirges/Kristallin	0,3		1
10P1.2	permische Sedimente	341,2	19	1
10P1.3	permische Vulkanite	15,8		1
10P1.4	sedimentäres Paläozoikum	51,7		1
10P2.1	saure bis intermediäre Silikatgesteine des Kristallinen Grundgebirges	2270,5	23	3
10P2.2	präkambrische bis paläozoische Metamorphite	1857,6	3	1
10P2.3	sedimentäres Paläozoikum	12,4		1
10P2.4	proterozoische bis präkambrische Metakarbonate	0,4		1
10V1.1	tertiäre Vulkanite	1,4		1
11G	Gewässer	322,4		1
11K1	Quartär, anthropogen (Tagebaubereiche)	501,8		2
11kA	nicht bewertet	177,5		47

* HGC areas of hydrogeological region 1 were derived from hydrogeological sub-regions