

Resources of groundwater, harmonized at Cross-Border and Pan-European Scale

Deliverable 3.3

3D visualisation of groundwater composition and age

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Version: draft

This report is part of a project that has received funding by the European Union's Horizon 2020 research and innovation programme under grant agreement number 731166.



Deliverable Data			
Deliverable number	D3.3		
Dissemination level	Public		
Deliverable name	3D visualisation of groundwater composition and		
	age		
Work package	WP3, H3O-PLUS		
Lead WP/Deliverable beneficiary	VMM		
Deliverable status	•		
Submitted (Author(s))	21/05/2021	Mariëlle van Vliet	
Verified (WP leader)	23/05/2021	Cis Slenter	
Approved (Coordinator)	27/05/2021	Hans Peter Broers	





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1 INTRODUCTION

The cross-border demonstration project H3O-PLUS intends to set a new standard for harmonization across borders, not only for hydrostratigraphy, but also for hydrological data such as groundwater heads and groundwater quality.

H3O-PLUS, WP3 of GeoERA RESOURCE, aims to be an advanced demonstration of a transboundary assessment of groundwater resources. It is 'advanced' in the sense that it builds on and extends on previous work, trying to make it more useful for groundwater policy and management and for subsurface spatial planning. A 3D hydrogeological model has been developed in a series of so called 'H3O' projects¹ in the transboundary region around the Roer Valley Graben, comprising parts of Germany, the Netherlands and Belgium (Vernes et al. 2018). The model contains 3D maps of the top, base and thickness of aquifers and aquitards. H3O-PLUS aims to add attribute data to these maps to facilitate the use of the maps in decision making processes. Note that the project does not aim to produce new maps or spatial delineations. The objective is to characterize units on existing maps and hence support the interpretation and use of those existing maps.

The overall study area coincides with the study areas of previous H3O projects (Figure 1.1). Vertically, the study is limited to the clastic (hydro)geological layers of Cenozoic age or younger. This coincides with the vertical scope of the recently developed transboundary 3D (hydro)geological models of the H3O projects. The base of the models is thus located at the top of the Chalk aquifer (Houthem, Maastricht / Kunrade Formation) or the top of the Carboniferous deposits.

¹ For more information and data downloads of the H3O-projects, the reader may refer to <u>H3O</u> (H3O website of TNO), <u>H3O-Roerdalslenk (website of the Flemish administration)</u>, or <u>H3O-De</u> <u>Kempen (website of the Flemish administration)</u>.







Figure 1.1: Study areas of previous H3O projects (note the label "Roerdalslenk" can be translated to "Roer Valley Graben")

This report describes the set-up and functioning of the GeoERA Groundwater Quality Viewer. The initial Dutch version of Groundwater Quality Viewer (www.grondwatertools.nl/gwatlas) has been the result of a pilot in which a method has been developed to disclose information about groundwater quality. This pilot was carried out for the central Dutch Rhine and Meuse river valleys, for which groundwater quality data were previously collected. This initial Dutch version has been expanded and new features were added. In the special GeoERA version data of the provinces Noord-Brabant and Limburg, Flemish data from VMM and SCK and German data (North Rhine-Westphalia) have been added. Groundwater Quality Viewer is a product of the Geomodelling department of the Geological Survey of the Netherlands, part of TNO. The application shows data that has been processed, averaged over time and, if applicable, over the depth trajectory.

The work has been supported in part by the Dutch provinces of Noord-Brabant and Limburg, as well as the water companies Brabant Water and WML.





2 METHODOLOGY

2.1 Data description

2.1.1 Groundwater quality data

All available time series data were collected both within the H3O-PLUS area and within the rest of the Dutch provinces of Noord-Brabant and Limburg. All available parameters were requested. At least the following parameters are required to carry out tests for quality control and quality assurance: Ca, Mg, Na, Fe, K, HCO3, SO4, Cl, NO3, Al, pH, EC. The data can be accessed with the GeoERA groundwater quality viewer. The viewer does not show raw data, but processed data, quality tested and averaged over time and, if applicable, over a user defined depth trajectory.

Data GDNRW

In Germany, a water quality database is available, but this is not managed by Geologischer Dienst Nordrhein-Westfalen (Geologischer Dienst NRW). Data was extracted from the HygrisC database, which is managed by LANUV

(https://www.lanuv.nrw.de/umwelt/wasser/grundwasser/grundwasserstand/grundwasserdat en-online). Geologischer Dienst Nordrhein-Westfalen extracted this data and sent them to TNO. Spring data is not included in the viewer.

Data VMM

In Flanders, all data was collected by VMM, are publicly available. The raw data is publicly accessible through <u>Portaal (vlaanderen.be)</u>. For this project, data is delivered in three separate data files:

- Fys_chem.csv
- Zware_metalen.csv
- Anionen_Kationen.csv

After a few quality checks, data is merged into one VMM dataset for further use in the Groundwater Quality Viewer.

Data SCK

Project partner SCK (www.sckcen.be/en/) delivered two datasets. One of these sets contains confidential data. This confidential data is not included. Only data from SCK_deep_wells.xlsx is imported to the viewer.

Data TNO

In the Netherlands data is derived from:

- Data and Information on the Dutch Subsurface ('DINO-metingen' and 'DINO-analyses'). This database is managed by TNO (https://www.dinoloket.nl/en),
- Data of provincial groundwater quality network of the Provinces Noord-Brabant and Limburg.

Data Brabant Water

Brabant Water is the supplier of drinking water in the province of Noord-Brabant. Brabant Water delivered data from observation wells but not from pumping wells to the GeoERA Groundwater Quality Viewer. Data from the catchment areas of the drinking water abstractions of Veghel and





Seppe have yet been added to the viewer, but more data is expected to be delivered before the end of GeoERA.

2.1.2 Groundwater age data

Information about the age of the groundwater has been collected through time and was brought together for the H3O-PLUS pilot area. Most of the available data was collected before 1990 and was stored in the DINO database or collected in cooperation with the University of Groningen. SCK delivered a number of samples for the Belgian part of the study area from their database. For the 3D viewer, we used the available data on ¹⁴C_{DIC} and ¹³C_{DIC} to interpret the "¹⁴C apparent age". In calculating the ¹⁴C apparent age, we corrected for the dilution of ¹⁴C of infiltrating soil CO_2 by dead carbon that is present in the form of carbonates in the subsurface. For the pilot region, the assumption was made that carbonate dissolution happened under closed system conditions, which is valid as the upper part of the subsurface is free from carbonates. We applied the concept of Han & Plummer (2016) for deriving zero-age lines, as depicted in Figure 2.1. Based on the position of a groundwater sample in the groundwater system and the geological formation, we used different zero-age lines for determining the ¹⁴C apparent age. When either the ${}^{13}C_{DIC}$ or the $\delta^{18}O$ indicated that the formation of methane had influenced the ${}^{14}C$ evolution history, we preferred the zero-age lines for infiltration under a peat bog or the zero-age line for methane formation by deep methanogenesis, depending on the hydrogeological position and the geographical position.



Figure 2.1 Example of applying the Han-Plummer approach for samples of the Waalre Formation.

In the groundwater viewer, the groundwater ¹⁴C apparent ages (in years) are available as a separate parameter and are displayed in the same way as other (chemical) parameters.

2.1.3 Hydrogeology data

For the H3O-PLUS area, geology and hydrogeology data is taken from the H3O projects (Deckers et al., 2014; Vernes et al., 2018; Vernes et al., in prep.; Kruisselbrink et al., in prep). For the remaining area of the Dutch provinces of North Brabant and Limburg, DGM's geological models (Hummelman et al., 2019a) and REGIS II v2.2 hydrogeological models (Hummelman et al., 2019b) have been attached to the models of the H3O-PLUS area.





2.2 Coordinate system and reference level

The original data has been delivered in coordinates from the systems used in the partner countries:

- Belgium: Lambert
- Germany: UTM
- the Netherlands: RD

The Belgian and German coordinates have been converted to the system from the Netherlands (RD) as a common system for H3O-PLUS. The 'GeoERA Groundwater Quality Viewer' also works with RD. Water quality data of other regions were added in the GeoERA Groundwater Quality Viewer during the H3O-PLUS project. TNO carried out the coordinate transformation into RD of all data that were shared by the project partners.

The reference level for elevation is based on the system that is used in the Netherlands (NAP). Belgian data is provided to TNO in mTAW and TNO was responsible for converting this to NAP level. With Germany, no conversion is required as both the German and the Dutch references correspond with the average sea level.

2.3 Data processing and quality control

The GeoERA Groundwater Quality Viewer contains a tool for data processing. When reading a dataset, a number of automatic checks are performed by the tool:

- check on mandatory metadata (coordinates, well name, screen number, screen depths, sampling date)
- consistency checks (coordinates, surface level, screen depths)
- screen depths checks (screen depths below surface levels, top screen above bottom screen)
- duplicates (same well-screen-date)

The tool also assigns the following properties to filters:

- time period:
 - o past-1980
 - o 1980-present
 - depth trajectories:
 - >+5 m+NAP
 - +5 tot -10 m+NAP
 - -10 tot -25 m+NAP
 - -25 tot -55 m+NAP
 - <-55 m+NAP
- geological layers based on H3O (Deckers et al., 2014; Vernes et al., 2018; Vernes et al., in prep.; Kruisselbrink et al., in prep) and DGM ('Digital Geological Model') (Hummelman et al., 2019a)
- hydrogeological layers based on H3O (Deckers et al., 2014; Vernes et al., 2018; Vernes et al., in prep.; Kruisselbrink et al., in pre) and REGIS II v2.2 ('REgional Geohydrological Information System') (Hummelman et al., 2019b)
- land use (based on CORINE Land Cover, 2018)





Furthermore, the tool has some automatic data quality checks for the consistency of various parameters in an individual water sample (Berendrecht, 2020):

- ion balance;
- pH vs Al;
- pH vs Zn;
- pH vs Cd;
- pH vs Cu;
- pH vs Ni;
- pH vs As;
- pH<3,5 or pH>10;
- Fe vs NO3 (screen <3 metre).

Users of the GeoERA Groundwater Quality Viewer can choose whether or not the less reliable data are shown.

However, values with a too high detection value will be removed and not shown on the website. More information about the checks can be found in Berendrecht (2020).

The tool derives a number of non-numerical parameters that are included in the viewer:

- water type
- pH class
- calcite saturation
- oxidation capacity class
- salinity
- redox classification

For the parameters water type, pH class, calcite saturation, oxidation capacity class, and salinity, the classification is taken from Graf Pannatier et al. (2000). The redox classification is based on Graf Pannatier et al. (2000) who created it for the Dutch National Monitoring network (LMG), but with some recent changes in order to make it more generally useful for multiple datasets (see GeoERA HOVER reports Broers et al., 2020 and Pinson et al., 2020).





3 DESCRIPTION OF THE GEOERA GROUNDWATER QUALITY VIEWER

3.1 Introduction

The GeoERA Groundwater Quality viewer can be accessed via the following link: <u>https://www.grondwatertools.nl/gwatlas/login</u>

A username and password are requited for access, as the tools is still under continuous construction. This will no longer be necessary after the official release at the end of the GeoERA project period.

The GeoERA Groundwater Quality viewer contains Flemish, German and Dutch data. This makes it possible to visualize and analyse cross-border variation in groundwater quality. The tool offers a 'static' view on groundwater quality, showing average concentrations over rather long time ranges. Time series and trends are not part of the current version of the viewer. Raw data is not shown.

Short description of functionalities

The available data is subdivided into three periods that can be chosen by the user (pre-1980, past-1980, periods combined). The viewer will only show the measurements that fall within this chosen time period. Measured values within a period are aggregated per measuring point to obtain a time-averaged value. The option Combined displays the value for the most recent time period available for each location.

Data can be displayed in three different ways:

- Depth trajectories: show parameters per trajectory. These trajectories divide the subsurface into layers of equal NAP depth. For each measurement location, the measurement values are averaged over a depth trajectory. Once you have selected a trajectory and parameter, the corresponding parameter values appear in the map. You may then use the button 'Charts' at the top of the menu bar visualize the data in different charts.
- Formations: View parameters per geological formation. Data can also be classified on the basis of geological formations as defined within the H3O-projects and DGM. You can then use the button 'Charts' at the top of the menu bar visualize the data in different charts.
- Cross section: view parameters in a cross section. Once you have opened the tab Cross section, the button
 appears at the top left of the map. If you click on this, you can draw a line, along which a cross section is then compiled.

Generating charts

With the button Charts at the top of the menu bar you can visualize the selected data in different charts. The following graphs are available:

- Boxplot
- Frequency distribution
- Histogram (non-numerical parameters)
- Depth plot





3.2 Features of the GeoERA Groundwater Quality Viewer

In this paragraph the application is explained by using examples in the H3O-PLUS project area. First, go to <u>https://www.grondwatertools.nl/gwatlas/login</u> and type username and password (*Figure 3.1*). The password is available for registered users: please contact marielle.vanvliet@tno.nl for registration.

Log in	
La GeoEra	
· ····	
Login	
	Log in

Figure 3.1 Log in screen

Second, choose a parameter and depth trajectories (*Figure 3.2*). In the example below, we choose to select all trajectories and the parameter Sulphate. On the map all available measurements appear. As a background map we choose 'Topography color'. Default you will see the grey topography map.



Figure 3.2 Available sulphate measurements for 5 selected depth ranges

Another possibility is to select groundwater quality data by Formation (*Figure 3.3*). Below, the Formations of Beegden, Sterksel, and Oosterhout were selected.







Figure 3.3 Sulphate parameters for 3 selected formations

Data can be analysed using various charts. Go to 'charts' and select, 'current view' to analyse all the data shown on the map. Below, boxplots are shown for Formations of Beegden, Sterksel and Oosterhout. This chart shows that the sulphate concentration of the Formation of Oosterhout is lower than the concentrations in the Sterksel and Beegden Formations (*Figure 3.4*). The outliers of these two formations are much higher than in the Formation of Oosterhout.



Figure 3.4 Boxplots

It is then easy to switch to the other chart types: frequency distributions and depth plots (see *Figure 3.5* below). In the depth plots, concentration per formation is plotted against depth. The figure below shows that the Oosterhout Formation extends to greater depths and - except for extreme values - has lower sulphate concentrations. A formation can be turned on and off by clicking on the formation name in the legend. It is also possible to draw the Lowess (Locally Weighted Scatterplot Smoothing, Cleveland, 1981), a smooth curve through the data that shows the relation between the concentrations and depths.







Figure 3.5 Depth plot for sulfate per formation

Finally, groundwater quality can be analysed using cross sections. After drawing a line on the map, click on 'show cross section' (*Figure 3.6*).



Figure 3.6 Drawing a cross section

The cross section below (*Figure 3.7*) shows the sulphate parameter values with depths along the line from 's Hertogenbosch to Aachen. The direction in which the line has been drawn determines how the cross section is shown. The background shows a hydrogeological model of the subsurface, providing insight into the relationship between parameter values and occurring hydrogeological layers. The cross section is interactive. The user may zoom in, get more information about data by hovering over the cross section, and add or remove additional data. The user may turn off and on the extraction wells (transparent grey). The same may be done for the zone for which the estimated travel time of groundwater from/to the surface level is less than 60 years ('< 60 years from slvl'), for the zone for which the estimated travel time of groundwater from/to the surface level is between 60 and 200 years ('60-200 years from slvl') and for the line that shows the estimated depth of the brackish-salt water interface (1000 mg/l isochlor).







Figure 3.7 Cross section from 's Hertogenbosch (north) to Aachen (south). Please not that the section extends from Germany on the right to the Dutch Meuse river valley to the left

The cross-section height can be changed with the slider 'cross section height'. By moving the mouse over the cross section, a tooltip appears containing the name of the hydrogeological layer or as soon as the mouse hovers over a measurement, the value and depth of the measurement appears (*Figure 3.8*).



Figure 3.8 Cross section with adjusted section height





Another possibility is to adjust the viewing depth of the measurements to show fewer / more measurements in the cross section. By default, a 1500 m buffer is used on both sides along the cross-section line (*Figure 3.9*). The cross section can be zoomed in along the horizontal axis by selecting the zooming area with the mouse (see blue area in *Figure 3.9*). *Figure 3.10* shows the result where the height of the cross-section is also set to a smaller value.



Figure 3.9 Cross section with adjusted viewing depth of the measurements and mouse selecting an area to zoom in along the horizontal axis.



Figure 3.10 Cross section zoomed in along the horizontal axis.





Figure 3.11 shows a newly drawn cross-section over the H3O-PLUS area from southwest to northeast. In this cross-section, the Campine block, Roer Valley Graben and Peel block become visible. The purple layer is the Boom Formation, a low permeability marine clay layer.



Figure 3.11 Cross section showing Campine Block, Roer Valley Graben and Peel Block.

After adjusting the height of the cross section, zooming and selecting the redox class parameter, the following cross-section (*Figure 3.11*) is shown. The cross section shows oxic/suboxic groundwater (red color), containing nitrate, in the upper layers. The redox transition from Fereduced (light orange) to Sulfur-reduced/methanogenic (light blue) is visible downwards.



Figure 3.12 Cross section showing redox transition from oxic/suboxic to Sulfurreduced/methanogenic.





In the groundwater viewer, the groundwater ¹⁴C apparent ages (in years) are available as a separate parameter called 'Carbon-14 apparent age' and are displayed in the same way as other (chemical) parameters. *Figure 3.13* shows the carbon-14 apparent age in a cross-section from north to south of the H3O-PLUS area. In the northern part, the carbon-14 apparent ages are older than in the other part of the area shown in the cross-section. In the southern area, the cross-section shows that deeper groundwater has a higher Carbon-14 apparent age. *Figure 3.13 Cross-section showing Carbon-14 apparent age (years)*



Figure 3.13 Cross-section showing Carbon-14 apparent age (years).





4 CONCLUSION

Groundwater quality data in the Roer Valley Graben areas has been processed and made available in the GeoERA Groundwater Quality Viewer. The data has been provided by German, Belgian and Dutch project partners. The Quality Viewer is accessible through https://www.grondwatertools.nl/gwatlas/geomap/era?language=en but requires a password and registration as a user until the end of the GeoERA project. The link to the Viewer will be available through EGDI, the European Geological Data Infrastructure (http://www.europegeology.eu/)





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