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Research paper

# AkvaGIS: An open source tool for water quantity and quality management

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## ABSTRACT

AkvaGIS is a novel, free and open source module included in the FREEWAT plugin for QGIS that supplies a standardized and easy-to-use workflow for the storage, management, visualization and analysis of hydrochemical and hydrogeological data. The main application is devised to simplify the characterization of groundwater bodies for the purpose of building rigorous and data-based environmental conceptual models (as required in Europe by the Water Framework Directive). For data-based groundwater management, AkvaGIS can be used to prepare input files for most groundwater flow numerical models in all of the available formats in QGIS. AkvaGIS is applied in the Walloon Region (Belgium) to demonstrate its functionalities. The results support a better understanding of the hydrochemical relationship among aquifers in the region and can be used as a baseline for the development of new analyses, *e.g.*, further delineation of nitrate vulnerable zones and management of the monitoring network to control chemical spatial and temporal evolution. AkvaGIS can be expanded and adapted for further environmental applications as the FREEWAT community grows.

## 1. Introduction

Environmental assessment and characterization of groundwater bodies (as required by the Water Framework Directive; European Commission, 2000) involve continuous monitoring and evaluation of a large number of physical and chemical parameters (*e.g.,* groundwater level, temperature, pH, or nitrates, among others). These parameters, which are used to conceptualize the behaviour of the environmental system, can be reinforced by other information (such as geology or isotopes) and are often stored in different scales and formats (*e.g.,* maps, spreadsheets or databases). This conceptualization of the environment is essential for the development of numerical models (Refsgaard et al., 2010), which are common and effective tools used to obtain deeper insights into physical systems. For instance, groundwater numerical models supported by hydrochemical data are used to (i) control different flow paths and their relationships among different water bodies, (ii) characterize water-rock interactions, (iii) identify water quality spatial and temporal evolutions, (iv) evaluate groundwater storage changes, and (v) design strategies to achieve a good chemical status based on national/international thresholds for water quality, among others. With respect to the latter, water agencies, stakeholders and water suppliers usually encounter difficulties in ensuring compliance with standard regulatory guidelines (Gleeson et al. 2012; Jurado et al., 2017; Vázquez-Suñé et al. 2006, 2016).

Geographical Information Systems (GIS) provide useful tools for addressing the abovementioned issues in collection, archiving, analysis, and visualization of spatial and non-spatial data in different formats. GIS software is widely used by the scientific community, public administration and the private sector. The comprehensive application of GIS platforms may aid in producing environmental assessments such as evaluation of water quality, water availability, zone mapping and risk assessment from the local to regional scale (Duarte et al., 2018; Ghosh

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et al., 2015; Tiwari et al., 2017) and improving numerical modelling processes (Kresic and Mikszewski, 2012; Rios et al., 2013; Rossetto et al., 2013; Steyaert and Goodchild, 1994), among other applications.

Several authors have developed GIS techniques within licensed GIS platforms to optimize environmental analyses (*e.g.*, Chenini and Ben Mammou, 2010; Kim et al., 2012; Lee et al., 2018) and address groundwater quality issues (*e.g.*, Ashraf et al., 2011; Babiker et al., 2007; Marchant et al., 2013; Nas and Berktay, 2010). These broadly applied advancements were mostly developed in commercial GIS platforms, the commercial licence of which is an obstacle for communities/institutions with limited resources, and these entities are consequently unable to benefit from this technology. Additionally, certain of these developments are not open source, and thus they cannot be expanded and/or adapted for tailored or further applications by third parties. However, these efforts have approached common conceptual and technical issues through creation of GIS-based tools related to (i) management and integration of a notably large amount of time-dependent and spatially dependent data (Cabalska et al., 2005; Chesnaux et al., 2011; Gogu et al., 2001; Maidment, 2002; Strassberg, 2005; Velasco, 2013; Wojda et al., 2006); (ii) homogenization and harmonization of data collected from diverse sources obtained with different techniques (De Dreuzy et al., 2006; Létourneau et al., 2011; Romanelli et al., 2012); (iii) communication and data exchange in different formats (Kingdon et al., 2016; Wojda and Brouyère, 2013); (iv) management of hydrological, geological, hydrogeological and hydrochemical data with diverse temporal and spatial ranges (Criollo et al., 2016; Merwade et al., 2008; Vázquez-Suñé et al., 2016; Velasco, 2013; Velasco et al., 2014); and (v) analysis of the required spatio-temporal data oriented to pre- and post-processing and generation of hydrogeological models (Alcaraz et al., 2017; Li et al., 2016; Strassberg et al., 2011; Wang et al., 2016).

Given these obstacles, the need becomes clear for open-source and user-friendly software that allows free access to the groundwater community for both application and further developments to adapt these tools to specific institutions and/or third-party databases (Bhatt et al., 2014; Dile et al., 2016). Specific open-source GIS-based tools are available that address these requirements for other topics, such as aquatic ecosystems assessments (Nielsen et al., 2017), which are beyond the scope of the current study but can be found in Khosrow et al. (2012); Ye et al. (2013); Teodoro (2018) or Huang et al. (2018). For groundwater management, open-source and GIS-based tools designed without specific user-friendly tools for hydrochemical and hydrogeological analyses in a unique GIS platform were developed to homogenize, integrate and visualize groundwater-related data (Boisvert et al., 2007, 2012; Jarar Oulidi et al., 2009, 2015) and to connect GIS platforms with groundwater numerical models (Bhatt et al., 2008, 2014; Carrera-Hernández et al., 2008; Rossetto et al., 2013). Hence, new open-source GIS-based software should allow standardization, management, analysis, interpretation and sharing of hydrogeological and hydrochemical data within a unique geographical context.

To address all of the aforementioned issues, a unique free and open-source GIS-integrated environment for water resource management with special reference to groundwater was developed in the context of the H2020 FREEWAT project (www.freewat.eu). The main objective was to promote the application of EU (WFD; European Commission, 2000) and other water-related directives (De Filippis et al., 2017; Foglia et al., 2018; Rossetto et al., 2015; Rossetto et al., 2018). FREEWAT is a large QGIS plugin (QGIS Development Team, 2009) (Fig. 1) in which all data related to surface and subsurface water bodies can be digitised, archived, analysed (also using integrated numerical models) and visualized. Additionally, the FREEWAT concept aimed to perform extensive capacity-building activities in an innovative participatory approach by gathering technical staff and relevant stakeholders for proper application of water policies (Criollo et al., 2018a; De Filippis et al., 2018; Foglia et al., 2017).

In this paper, we present the AkvaGIS tool, a user-friendly, free and open-source GIS-based package integrated into the FREEWAT platform (Fig. 1). AkvaGIS has been designed to fulfil the needs for (i) managing and visualizing hydrogeological and hydrochemical standardized data with different temporal and spatial scales to facilitate development of the environmental conceptual model, (ii) integrating data from diverse sources gathered using different data access techniques and formats, and (iii) preparing hydrogeological input files for any groundwater numerical model in all of the available formats in QGIS. Due to its open-source architecture, AkvaGIS can be updated and extended by any advanced user.

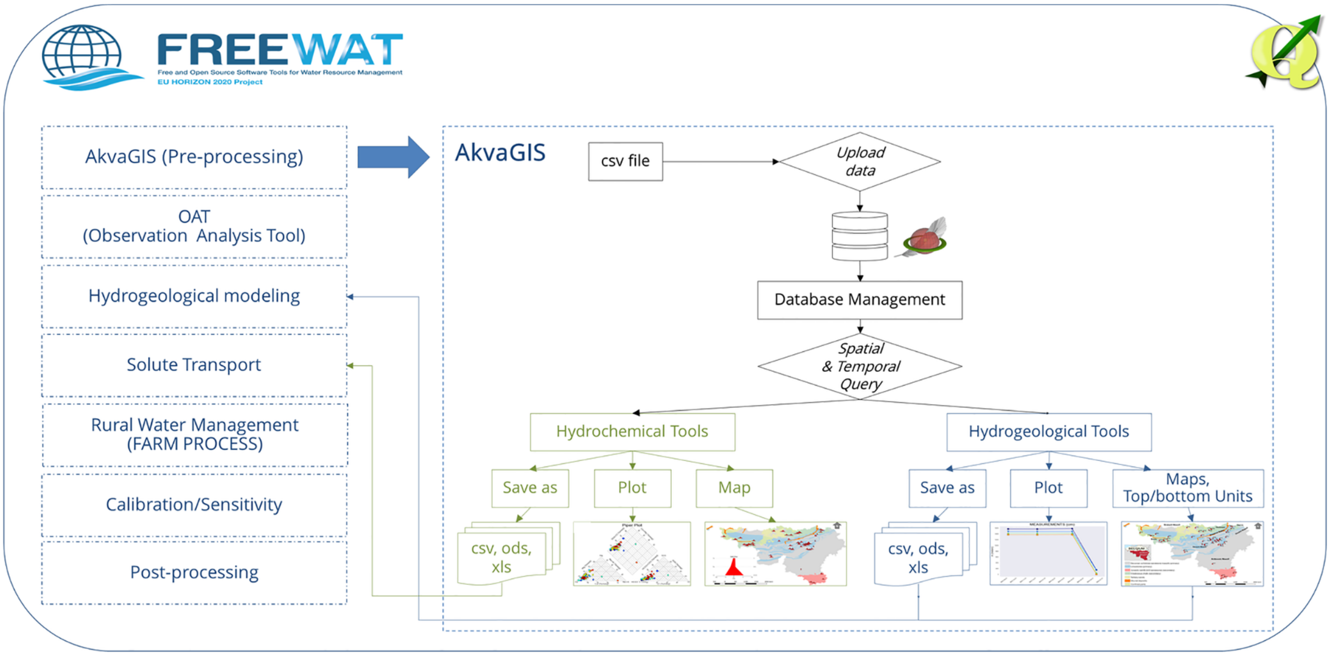


**Fig. 1.** AkvaGIS tools: Scheme of simplified workflow together with all FREEWAT tools. Colours correspond to the 3 main groups of tools: database management (black), hydrochemical tools (green) and hydrogeological tools (blue).

After a description of the AkvaGIS design and relevant tools in the following section, we present an application in the Walloon region (Belgium) to demonstrate certain capabilities. Finally, the development, the application and future improvements are discussed.

## 2. AkvaGIS description

AkvaGIS is the evolution of work performed by Velasco (2013), Velasco et al. (2014), Alcaraz (2016) and Criollo et al. (2016). In those studies, tools for geological, hydrochemical, geothermal and hydrogeological data analysis were developed in the commercial GIS desktop software ArcGIS (ESRI, 2004, 2012). Conversely, AkvaGIS is a free and open-source GIS-based tool supported in Linux and Windows OS and integrated in QGIS (Criollo et al., 2017). QGIS is supported by most operating systems (Windows, Linux, Unix, Macintosh) and has several data reading and writing formats. The data management subsystems allow easy and rapid queries that are quickly processed and displayed, and this tool has a large community of developers (Chen et al., 2010; Bhatt et al., 2014).

### 2.1. Software design and structure

AkvaGIS is developed in Python (www.python.org) and integrated into the FREEWAT platform (Fig. 1). This tool is freely available from the official QGIS experimental repository, the FREEWAT project repository (www.freewat.eu) or the gitlab repository (https://gitlab.com/freewat). The AkvaGIS tools enhance FREEWAT with hydrochemical and hydrogeological data processing and analysis. AkvaGIS is designed to avoid code repetition to reduce errors and improve the code maintenance under the GNU Lesser General Public License v2.0 (GPL) or later. Different third-party libraries are applied with GPL, MIT license and BSD license types. The Python-related dependencies that AkvaGIS applies are the Qt version 4 Python wrapper (PyQt4), a Python 2D plotting library that creates quality figures in a variety of hardcopy formats and interactive environments across platforms (Matplotlib 1.5, ChemPlotLib 1.0, Openpyxl2.3, Odfpy 1.3, and Pyexcel 0.2). All of these libraries are automatically downloaded during FREEWAT installation.

AkvaGIS tools are divided into 3 main sections (Fig. 2): the database management tools that are designed to manipulate the hydrochemical and hydrogeological data stored in the AkvaGIS database; the hydrochemical tools for managing, visualizing, analysing, interpreting and pre-processing the hydrochemical data; and the hydrogeological tool. This package was developed to facilitate interpretation of hydrogeological information and hydrogeological units, which in turn is crucial in defining conceptual models and in modelling activities. The hydrochemical and hydrogeological tools allow creation of contour maps and further spatial operations. Additionally, thematic maps (*e.g.*, chlorides, piezometric maps or pumping rates) can be created for the selected points and time periods using different functionalities included in the AkvaGIS menu.

#### 2.1.1. AkvaGIS database

The core of the AkvaGIS tools is a geospatial database (Fig. 3) implemented using the relational database SpatiaLite (SQLite spatial extension, http://www.sqlite.org/), where all data related to a hydrogeological study are stored. SpatiaLite is an open-source database able to store many format files (*e.g.,* raster, shapefiles or cad files), and it can build-in spatial indices, which facilitate rapid searches over large areas. A SpatiaLite database can be safely exchanged across different platforms because its internal architecture is universally portable (Spatialite Development Team, 2011). Accordingly, this database can be expanded and/or adapted for future applications and can be continuously improved. No-installation and no-configuration are required before using the AkvaGIS database file within QGIS.

The AkvaGIS database architecture can store a large amount of spatial features and hydrochemical and hydrogeological temporal-dependent data and is designed for different methodologies and tools used by water professionals and managers to address groundwater management issues. AkvaGIS considers the aforementioned existing projects (*e.g.*, Strassberg, 2005; Wojda and Bouyère, 2013) and implements selected international standards to store and exploit hydrogeological

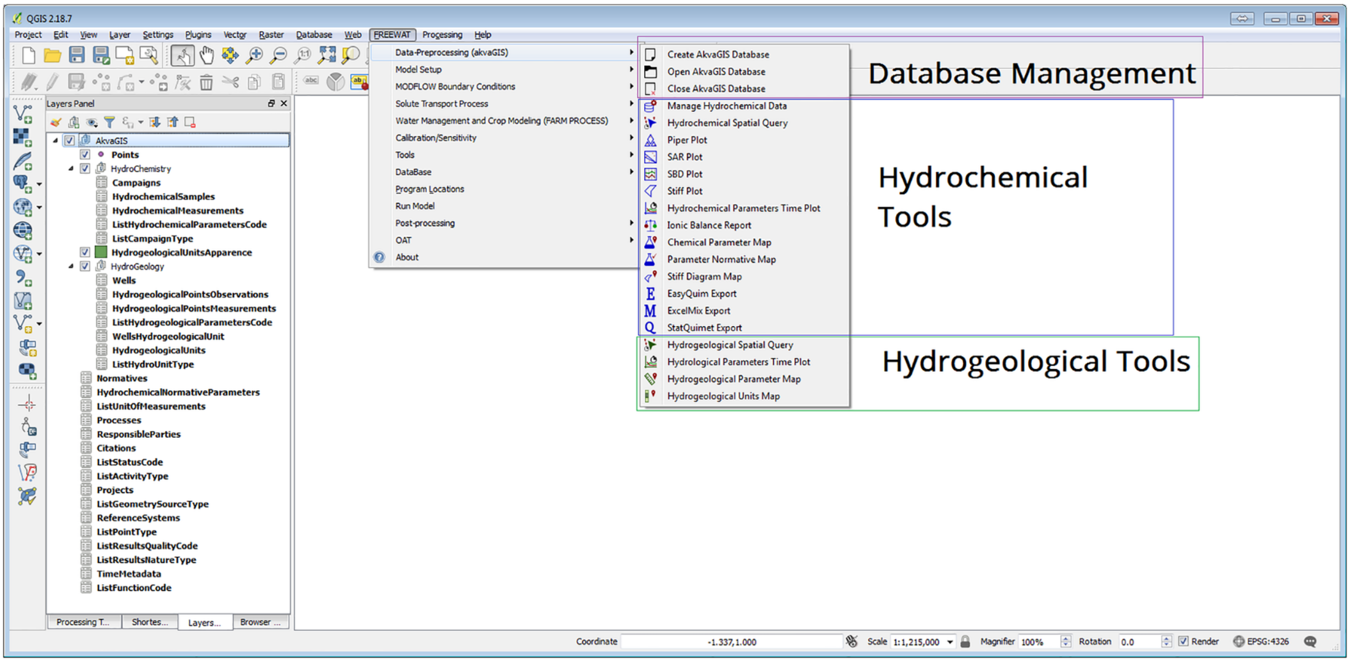


**Fig. 2.** FREEWAT menu of tools, including AkvaGIS tools, are presented in the QGIS layer panel (version 2.18 Las Palmas). AkvaGIS menu shows the three groups of tools: database management (black), hydrochemical (green) and hydrogeological (blue) analyses.

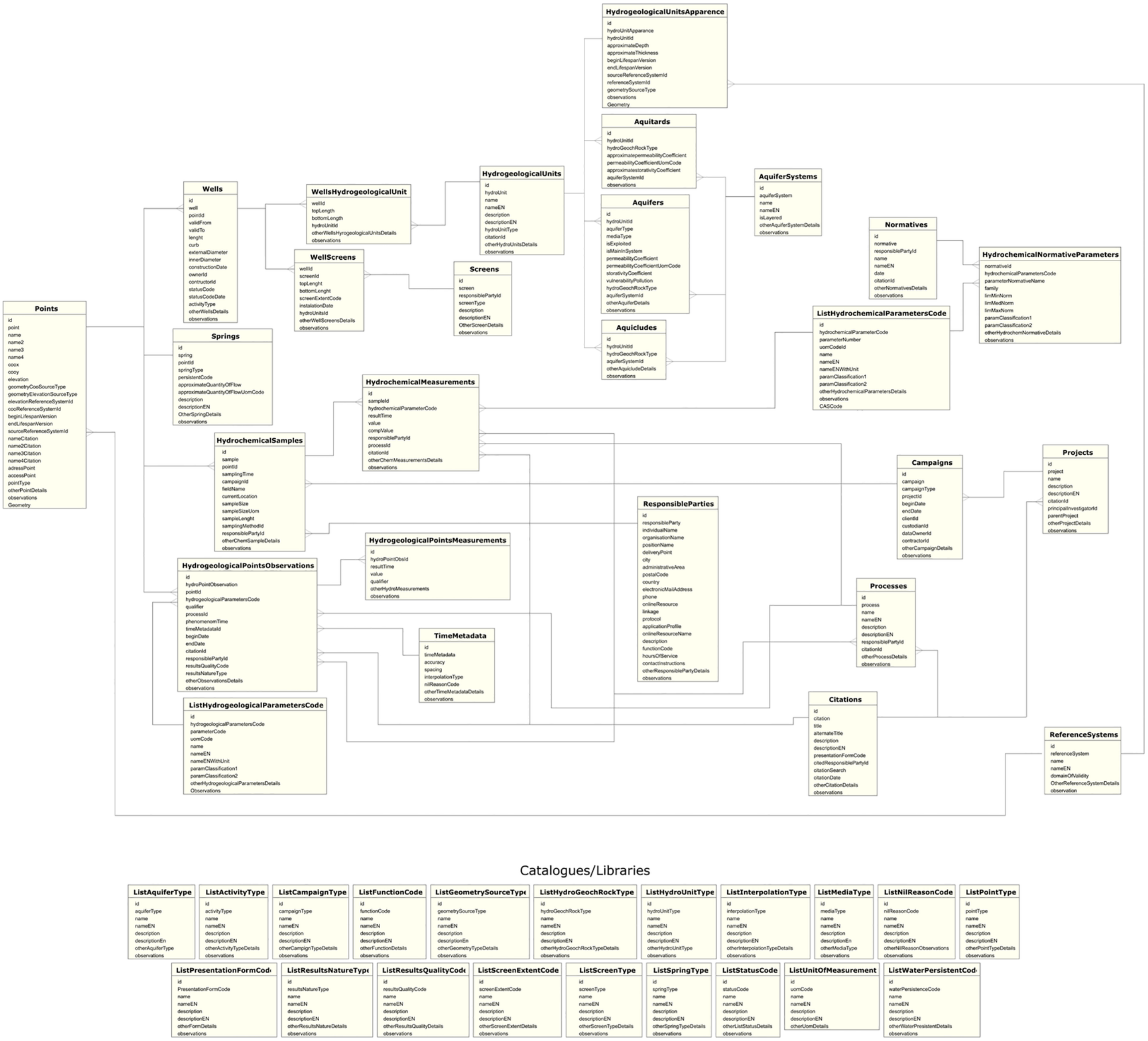


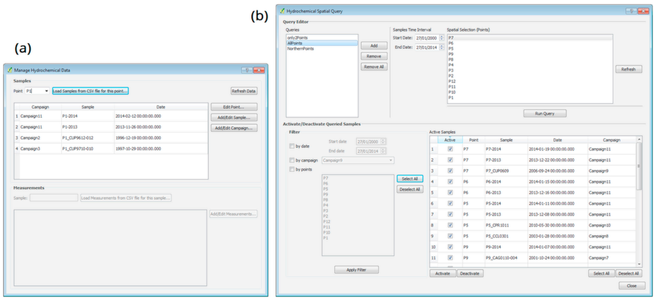
**Fig. 3.** AkvaGIS geospatial database scheme.

information, time series, and field observations and measurements. These standards are supported by the Open Geospatial Consortium (OGC, 2003, 2006; 2007; OGC Water ML 2.0, 2012), GeoSciML (Sen and Duffy, 2005), the specifications of the European Directive INSPIRE (INSPIRE, 2011, 2013) and the ONEGeology project (ONEGeology, 2013). Hence, the standardized architecture facilitates harmonization of the collected data, and the AkvaGIS database can be shared in a more understandable manner.

The spatial coordinates of the points (*i.e.*, piezometers, wells, springs, swallow holes, seeps, vanishing points or any other specific points from water bodies) related to the location of measurements/estimates or collected samples are the basic information required for use of the AkvaGIS tools and are stored in the *Points* table. The basic hydrochemical information related to each spatial point, i.e., *HydrochemicalSamples* and *HydrochemicalMeasurements* tables (Fig. 3), contains the dates when each named sample was collected, the dates of the physical and chemical parameters analysis, and their corresponding values and units. The list of analysed parameters is stored in a library/catalogue (*ListHydrochemicalParametersCode*) and can be updated by the user.

Similarly, the basic hydrogeological information is related to the corresponding spatial point at which the hydrogeological measures/estimates were collected. The measurement dates, measurements and estimated parameters and the corresponding values and units are stored in the tables *HydrogeologicalPointsObservations* and *HydrogeologicalPointsMeasurements*. The default hydrogeological parameters available in the library/catalogue *ListHydrogeologicalParametersCode* store flow rate, depth to water, pressure and hydraulic head. This list of parameters can be customized by the user. The hydrogeological unit observed at each point can be defined and stored in the tables *HydrogeologicalUnits* and *WellsHydrogeologicalUnit* (see Fig. 3). These interpreted units can be interpolated to generate surfaces of the boundaries of hydrogeological units of the study zone, which might be subsequently applied to define the three-dimensional geometry in groundwater numerical models. The created files can be saved in any format available in QGIS such as shapefile or raster.

Additional information can also be stored, such as field campaign number, entities in charge of measurements or responsible parties, among others. This information is not essential for use of the AkvaGIS tools, but it is useful in managing the hydrogeological and hydrochemical data. Detailed information on all AkvaGIS tables and their



Manage Hydrochemical Data

Samples

Point: P1

Load Samples from CSV file for this point... | Refresh Data

| | Campaign | Sample | Date |
|---|---|---|---|
| 1 | Campaign11 | P1-2014 | 2014-02-12 00:00:00.000 |
| 2 | Campaign11 | P1-2013 | 2013-11-26 00:00:00.000 |
| 3 | Campaign2 | P1_CUP9612-012 | 1996-12-19 00:00:00.000 |
| 4 | Campaign3 | P1_CUP9710-010 | 1997-10-29 00:00:00.000 |

Hydrochemical Spatial Query

Query Editor

Queries: only2Points, AllPoints, NorthernPoints

Samples Time Interval

Start Date: 27/01/2000

End Date: 27/01/2014

Spatial Selection (Points): P7, P6, P5, P9, P8, P4, P3, P2, P12, P11, P10, P1

Activate/Deactivate Queried Samples

Filter

☐ by date — Start date 27/01/2000, End date 27/01/2014

☐ by campaign — Campaign9

☐ by points — P7, P6, P5, P9, P8, P4, P3, P2, P12, P11, P10, P1

Active Samples

| | Active | Point | Sample | Date | Campaign |
|---|---|---|---|---|---|
| 1 | ☑ | P7 | P7-2014 | 2014-01-19 00:00:00.000 | Campaign11 |
| 2 | ☑ | P7 | P7-2013 | 2013-12-22 00:00:00.000 | Campaign11 |
| 3 | ☑ | P7 | P7_CUP0609 | 2006-09-24 00:00:00.000 | Campaign9 |
| 4 | ☑ | P6 | P6-2014 | 2014-01-15 00:00:00.000 | Campaign11 |
| 5 | ☑ | P6 | P6-2013 | 2013-12-16 00:00:00.000 | Campaign11 |
| 6 | ☑ | P5 | P5-2014 | 2014-01-11 00:00:00.000 | Campaign11 |
| 7 | ☑ | P5 | P5-2013 | 2013-12-08 00:00:00.000 | Campaign11 |
| 8 | ☑ | P5 | P5_CPR1011 | 2010-05-30 00:00:00.000 | Campaign10 |
| 9 | ☑ | P5 | P5_CCL0301 | 2003-01-28 00:00:00.000 | Campaign8 |
| 10 | ☑ | P9 | P9-2014 | 2014-01-07 00:00:00.000 | Campaign11 |
| 11 | ☑ | P9 | P9_CAG0110-004 | 2001-10-24 00:00:00.000 | Campaign7 |

**Fig. 4.** Using *Manage Hydrochemical Data* (Fig. 4a), tool users can update, upload or delete data stored in the AkvaGIS database. Diagram and maps are created by applying a *Hydrochemical Spatial Query* (Fig. 4b), which is subsequently stored in the same database for further analysis.

fields are shown in the FREEWAT user manual volume 4 (Serrano et al., 2017).

Through the QGIS project (.qgis file), the user manages the AkvaGIS database (.sqlite file) and additional files that are shown in the layer panel (see Fig. 2). The Database Management tools allow the user to create, open and close the AkvaGIS database (Fig. 3). Once the information collected is stored in the AkvaGIS database, users can apply the analysis tools.

### 2.1.2. Hydrochemical analysis tools

The Hydrochemical Analysis Tools package supplies a wide range of tools for performing hydrochemical data analysis through common queries and hydrochemical plots. The ***"Manage Hydrochemical Data"*** tool allows visualization of hydrochemical data from points already stored in the AkvaGIS database. The user can manage these data by adding, deleting or editing the needed information to perform the study (see Fig. 4a).

First, a selection query must be run to create diagrams and maps. This query is created and stored in the database for future application. The **"*Hydrochemical Spatial Query*"** tool performs a specific selection of points in the desired time period (see Fig. 4b). Selection using reference campaigns, dates or geographical position can be performed. Diagrams and maps preparation use the queries initiated with this tool. The query results can be saved in a table for further external analysis.

The ***"Ionic Balance Report"*** tool allows calculation of the ionic balance report (shown in Fig. 5a). This tool automatically converts all units to *meq/l* and selects the major ions of the chosen sample. Once the query is created, the user can save the results in a table or in an ionic balance report (.ods format).

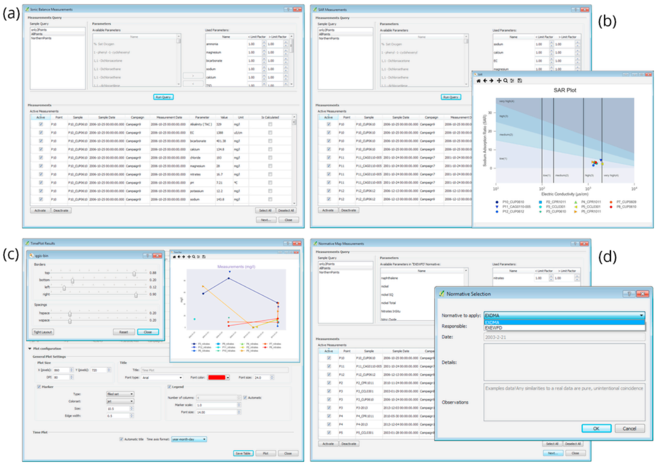


**Fig. 5.** Examples: Ionic Balance Measurements (5a); Sodium Adsorption Ratio diagram (5b); Time Evolution Plot (5c) and Normative Maps (5d).

AkvaGIS offers the ability to draw a number of hydrochemical diagrams useful for analysing the water chemical composition and how the collected samples relate to each other. The ***"Piper Plot"*** is useful for visualizing hydrochemical types of water samples classified by their ionic composition. The ***"SAR Plot"*** (Sodium Adsorption Ratio diagram, Fig. 5b) is useful for analysis of irrigation water quality to facilitate the management of sodium-affected soils. To visualize and analyse water mixing, end-members or changes between certain ionic relationships, users can apply the ***"Shöeller-Berkaloff diagrams"***. With the ***"Stiff Plot"***, the user can analyse the samples compositions in its spatial context among water from different sources. Fig. 5c presents the interfaces developed to manage these diagrams. Plot setup commands (plot size, point style, legend, among other configurations) are available in the AkvaGIS diagram and map tools.

Spatial analysis is useful in visualizing and analysing the hydrochemical spatial variation throughout the study zone. To this end, the ***"Chemical Parameter Map"*** and the ***"Stiff Diagram Map"*** tool supply spatial distribution analysis of the chemical samples and the Stiff diagram zone, respectively.

The temporal distribution of chemical parameters can be analysed by drawing a ***"Time Plot"*** of the query previously created using the *Hydrochemical Spatial Query* tool (Fig. 5c). In addition, tools are available to export the query data to different external platforms, for instance, for evaluation of common major ions (*e.g.*, Easy_Quim; Serrano and Vázquez-Suñé, 2014), mixing ratios of the samples (*e.g.*, MIX; Carrera et al., 2004) or ionic relationships and further statistical analyses (*e.g.*, Statistical Tools; Velasco et al., 2013).

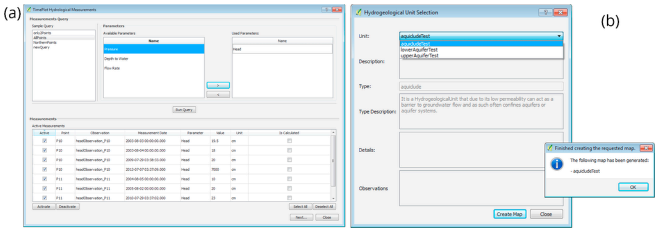
The ***"Parameter Normative Map"*** draws thematic maps according to the threshold values for the queried parameters established by a given guideline (*e.g.,* Water Framework Directive) (Fig. 5d). The guideline and their thresholds values must be uploaded and stored previously in the database by the user.

### 2.1.3. Hydrogeological analysis tools

This module presents a set of tools developed to improve management, visualization and interpretation of the hydrogeological data. The user can manage and query hydrogeological measurements and estimates performed in wells, piezometers or springs. Thematic maps of each chosen parameter (*e.g.,* piezometric maps) can be performed from the selected points and the specific time interval. General statistics can be calculated for each selected parameter to perform simple analyses of the temporal data. Additionally, this tool can simplify the construction of the geometry of groundwater flow numerical models. Hence, these tools create depth or thickness surfaces of the defined hydrogeological units (top and bottom of each layer). The user can save these structures in several formats with the QGIS tools and apply them in a groundwater numerical model (*e.g.,* MODFLOW).

Similarly, the ***"Hydrogeological Spatial Query"*** tool enables consultation of the hydrogeological measurements (*i.e.,* head level, water depth, pumping rates and discharge) collected in wells, piezometers or springs. This query only acts on those points where hydrogeological observations and measurements have been introduced in the database. This command creates and adds spatial queries of the selected points (spatial selection) for the desired time interval. Different methods are used to create this selection: by sampling campaigns, by dates or by the geographical positions. The interface uses the same commands as the hydrochemical spatial query interface.

In selecting the previously created desired hydrogeological spatial query, the user can create a time evolution plot of the chosen parameters using the ***"Hydrogeological Parameter Time Plot"*** tool (shown in Fig. 6a). Additionally, the ***"Hydrogeological Parameter Map"*** tool creates parameter maps of the selected query for the desired parameters. The available hydrogeological parameters are depth to water, flow rate, head or pressure (as listed in the library/catalogue *ListHydrogeologicalParametersCode*). The user is able to choose the value used in the map (earliest, latest, minimum, maximum or average) to draw



Sample Query: only2Points, AllPoints, NorthernPoints, newQuery

Available Parameters: Pressure, Depth to Water, Flow Rate

Used Parameters: Head

| Active | Point | Observation | Measurement Date | Parameter | Value | Unit | Is Calculated |
|---|---|---|---|---|---|---|---|
| ☑ | P10 | headObservation_P10 | 2003-08-03 00:00:00.000 | Head | 19.5 | cm | ☐ |
| ☑ | P10 | headObservation_P10 | 2003-08-04 00:00:00.000 | Head | 18 | cm | ☐ |
| ☑ | P10 | headObservation_P10 | 2009-07-29 03:38:33.000 | Head | 20 | cm | ☐ |
| ☑ | P10 | headObservation_P10 | 2013-07-07 03:37:09.000 | Head | 7000 | cm | ☐ |
| ☑ | P11 | headObservation_P11 | 2004-08-05 00:00:00.000 | Head | 10 | cm | ☐ |
| ☑ | P11 | headObservation_P11 | 2005-08-02 00:00:00.000 | Head | 20 | cm | ☐ |
| ☑ | P11 | headObservation_P11 | 2010-07-29 03:37:02.000 | Head | 23 | cm | ☐ |

Unit: aquicludeTest (aquicludeTest, lowerAquiferTest, upperAquiferTest)

Type: aquiclude

Type Description: It is a HydrogeologicalUnit that due to its low permeability can act as a barrier to groundwater flow and as such often confines aquifers or aquifer systems.

The following map has been generated:
- aquicludeTest

**Fig. 6.** Interface of the Time Plot Hydrogeological Measurements (6a) and Hydrogeological Unit maps (6b).

the most important information.

Three-dimensional groundwater flow numerical models require the definition of aquifer geometry. Therefore, a modeller must build surfaces limiting different hydrogeological units, as defined in the conceptual model. The ***"Hydrogeological Units Maps"*** tool (shown in Fig. 6b) creates maps of top/bottom hydrogeological units. Because the FREEWAT plugin includes MODFLOW (Harbaugh, 2005) as numerical code for groundwater flow simulation, the user can save these geometrical boundaries in a proper format for later implementation in a numerical model working in the same GIS environment.

For all tools described above, the results can be saved as tables, and the corresponding plots and maps can be user-customized. FREEWAT user manual volume 4 (Serrano et al., 2017) and the training material contain additional information on the AkvaGIS functionalities.

## 3. An example of AkvaGIS application: The Walloon region (Belgium)

Thus far, AkvaGIS and all of the FREEWAT tools have been extensively used by more than 1300 attendees during courses held in over 50 countries. The AkvaGIS tools have been further improved and developed to facilitate its handling because of the feedback supplied by these users.

In the following text, we present an application of selected AkvaGIS tools with real data to demonstrate the advantages of use. Specifically, AkvaGIS is applied to data collected in the Walloon region (southern region of Belgium-northwest Europe; Fig. 7). The Walloon region has an area of approximately 16,844 km$^2$, where half of the land is covered by agricultural areas and forests (approximately 30%) and urban areas (approximately 15%) (Brahy, 2014).

The Walloon region can be roughly divided into six main aquifer units characterized by geological age. Most aquifers are located in fractured rock systems that show a high degree of heterogeneity (Fig. 7). These aquifers can be distinguished by their degree of consolidation: (1) unconsolidated aquifers where groundwater is stored in the interstices of the subsoil (*e.g.*, Tertiary sands and Quaternarian alluvial deposits, Fig. 7) and (2) consolidated aquifers where groundwater is abstracted from permeable and fractured areas (*e.g.*, Primary limestones, Fig. 7) (SPW-DGO3, 2016).

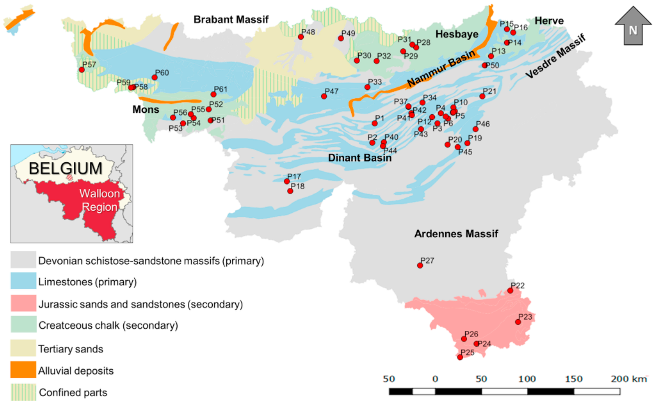


**Fig. 7.** Location of the study area (the Walloon region, Belgium) with the main aquifers. Sampling points are shown as red points.

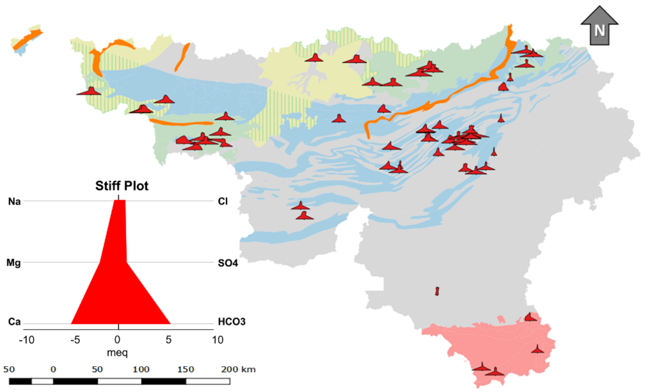


**Fig. 8.** Spatial distribution of the Stiff diagram of the Walloon region aquifers as generated from data collected in the 2016 campaign.

The majority of groundwater abstraction originates from limestone aquifers (51%, in blue) and chalky formations (21%) and is mainly applied for water supply purposes, representing up to 80% of the water volumes collected (400·10$^6$ m$^3$/y; SPW-DGO3, 2016).

A total of 64 groundwater samples were collected in spring 2016 within the framework of a project that investigated the occurrence and indirect emissions of greenhouse gases (GHGs) from groundwater at the regional scale (Jurado et al., 2018). Analysis of these samples included GHGs, major and minor ions and metals. Data from major and minor ions are used in this paper to display the functionalities of AkvaGIS. Database created for this purpose can be found in Criollo et al. (2018b).

After collecting and storing all of the data in the AkvaGIS database, the chemical analysis quality for charge balance was calculated. In total, 94% of the samples had less than ± 5% error (considered acceptable for this study). Once the hydrochemical data quality was ensured, the second step analysed the hydrogeochemical data using graphical diagrams. AkvaGIS generated a map presenting the Stiff plot for each sample. A quick review of this map shows that most of the groundwater samples could be classified as Ca-$HCO_3$ types (see Fig. 8).

These observations can be corroborated by generating Piper and Schoeller-Berkalof plots (Fig. 9). Although these plots do not provide supply information on spatial distribution, they allow identification of the main trends with respect to the chemical composition of water samples. The plots also show that most samples have a similar composition (Ca-$HCO_3$ type). However, it is possible to identify two samples with different compositions, *i.e.*, samples S51 and S27. Sample S51 has a high Na-$HCO_3$ concentration, and sample S27 is less mineralized but richer in potassium than the remainder of the samples. Note that the S24 sample (Jurassic sands and sandstones) is completely opposite of the previously described sample (Fig. 9b), with the lowest value of sodium and chlorides. The information derived from these plots is highly useful in defining the characteristics of aquifers (groundwater and rock chemical compositions should be related), residence times (the degree of mineralization might be related to the residence time) and/or potential uses (*e.g.*, water with high concentrations of Na$^+$ and low of Ca$^{++}$ is not advisable for irrigation purposes because it tends to reduce the permeability of the soil, IGME, 2002).

AkvaGIS tools also produce distribution maps for the nitrate concentration measured at different points. The nitrate concentrations show a strong spatial variability (see Fig. 10), especially in locations close to agricultural and farm areas. Furthermore, according to the Drinking Water Directive (European Commission, 1998), stored in the AkvaGIS database), the nitrate concentrations of 16% of the samples exceed the threshold value of 50 mg/l. These points are located in the Chalk zone, the most mineralized aquifer (908.6 µS/cm in the Chalk

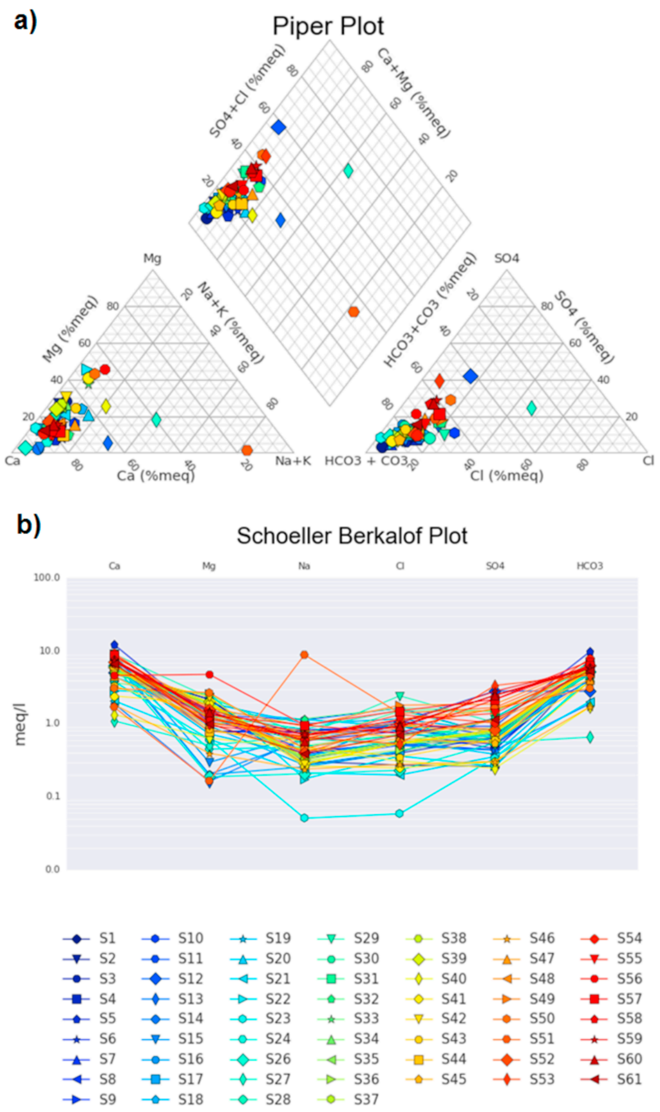


**Fig. 9.** (a) Piper and (b) Schoeller-Berkaloff diagrams of the sampling points from the spring 2016 campaign. Note that S27 and S51 samples have a stronger deviation with respect to the remainder of the samples.

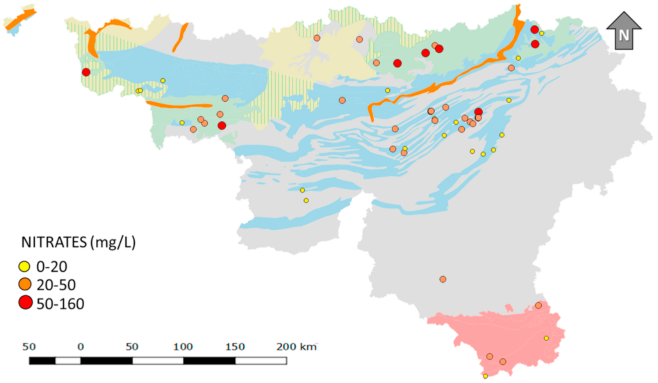


**Fig. 10.** Spatial distribution of the nitrate concentrations (mg/l) in groundwater for the spring 2016 campaign.

aquifer of the Hesbaye and 844.8 μS/cm in the Chalk aquifer of the Mons). Conversely, the Devonian limestones (shales and sandstones) of the Dinant Basin presented lower values of electrical conductivity, less than 430 μS/cm. The average dissolved oxygen concentrations showed that the groundwater had oxic conditions, ranging from 4 mg/L to 9.1 mg/L (see Table 1). Finally, the average temperatures presented little variation, varying from 10.2 °C to 13.4 °C.

The application of the AkvaGIS tools in the Walloon Region case study helped to (1) visualize and analyse data easily and quickly and (2) improve understanding of the hydrochemical relationships among aquifers in the region. These initial results might aid water resource authorities in design of future management and monitoring strategies to continue preservation of the quality and quantity of groundwater resources. For example, vulnerable zones due to high nitrate concentrations could be further delineated and the current monitoring network could be managed to control their spatial and temporal evolution using the AkvaGIS tools. The presented analysis can be extended to other regions for the same or other water analysis purposes (*e.g.,* hydrogeological modelling).

## 4. Conclusions

This paper presented the AkvaGIS GIS-based tool designed to improve the characterization of groundwater bodies, with specific reference to analysing the availability and chemical quality of groundwater. The AkvaGIS tool was developed within the context of the FREEWAT project to include relevant information on groundwater quality and hydrogeological information in analysis of water resources.

The user-friendly and GIS-based architecture of AkvaGIS is significantly standardized and supplies an easy-to-use workflow that can manage, visualize and analyse hydrochemical and hydrogeological data.

The AkvaGIS database structure ensures that all groundwater-related knowledge of a study area is archived and continuously updated without loss of the original information. Application of this tool can aid users in reinforcing the construction of conceptual models by cross-analysis of related data. In addition, AkvaGIS can simplify the preparation of input files for any groundwater numerical model in all of the available formats in QGIS.

An application of the AkvaGIS tools in the Walloon region (Belgium) demonstrated its usefulness by simplifying the steps needed to analyse the hydrochemical data. Use of analysis tools such as ionic balance analysis, Stiff maps, Piper diagrams, etc. facilitated understanding of the hydrochemical relationship among aquifers in the region and deduction of selected preliminary characteristics. This process represents a first step in further analysis of the region by the scientific community, public administration and the private sector for a wide range of environmental projects (*e.g.,* water supply, water quality control, mining control, among others).

In addition, these first observations might spur future strategies focused on continued preservation of water quality and quantity indices in the Walloon region.

AkvaGIS aims to endorse water management and planning by simplifying the application of water-related directives (*e.g.,* Water Framework Directive) focusing on groundwater bodies. The scientific community, water resource authorities, and the private sector might benefit from using AkvaGIS, thus reducing the costs of commercial software and improving open sharing of hydrochemical and hydrogeological data and its interpretations in the water governance process.

Due to its open-source architecture, AkvaGIS can be updated and extended depending on the tailored applications. The FREEWAT community ensures proper functionality of all tools, manuals and their training material. Further development will address hydrochemical and hydrogeological analysis from different aspects such as a better connection between AkvaGIS and the hydrochemical numerical models.

## Software availability

**Software name**: AkvaGIS (Version 1.0. September 2017).

**Availability**: AkvaGIS has been developed under the H2020 FREEWAT project. So AkvaGIS is included in the FREEWAT plugin for

**Table 1**
Average of the in-situ parameters of each aquifer.

| Aquifer formation | Aquifer ID | pH | DO (mg/L) | EC (µS/cm) | $T^a$ (°C) |
|---|---|---|---|---|---|
| Devonian schisto-sandstone massifs (shales and sandstones) | Ardenne Massif | 6.74 | 6.0 | 560.0 | 12.2 |
| | Dinant Basin | 7.59 | 6.4 | 552.5 | 10.8 |
| Primary limestones | Namur Basin | 7.19 | 4.0 | 788.7 | 13.4 |
| | Dev. Dinant Basin | 7.58 | 8.1 | 425.5 | 10.2 |
| | Carb. Dinant Basin | 7.21 | 6.4 | 732.9 | 11.0 |
| Jurassic formations (sands and sandstones) | Formations Sud Luxembourg | 7.51 | 4.7 | 521.6 | 10.5 |
| Cretaceous chalks | Chalks of Mons | 7.13 | 8.8 | 844.8 | 12.8 |
| | Chalks of Hesbaye | 7.49 | 8.4 | 908.6 | 13.2 |
| | Chalks of Pays de Hervé | 7.03 | 6.9 | 671.8 | 10.5 |
| Tertiary sands | Bruxellian and Landenian Sands | 7.37 | 9.1 | 736.0 | 11.1 |

QGIS. Software and documentation (user manual and training material) is freely available from the FREEWAT website (http://www.freewat.eu/download-information, accessed September 2018). Code source can be accessed through the gitlab H2020 FREEWAT project repository under the GNU Lesser General Public License v2.0 (or later). It can also be installed directly from the official QGIS repository of experimental plugins.

## Credit authorship contribution statement

VV, AN, LMV, EVS and RC designed and developed AkvaGIS; LS, CR and RC made figures and wrote the manuscript with input from all authors. AJ, EP and SB performed data acquisition. SB coordinated the project to obtain the hydrochemical information. AJ, EP with collaboration of LS performed the analysis of hydrochemical data using the software presented in this manuscript. RR, VV, RC and EVS coordinated the capacity building of more than 1300 people of FREEWAT (including AkvaGIS tools). Feedback obtained in these trainings helped to improve the software, manuals and training material. RR coordinated the FREEWAT project. All authors discussed results and edited the paper.

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