WaterJPI project

SMARTControl

Smart framework for real-time monitoring and control of subsurface processes in managed aquifer recharge (MAR) applications

Deliverable D4.1

Web-based real-time monitoring and control capabilities
Development and implementation of a web-based tool for the calculation of groundwater hydraulic residence time

Authors

Catalin Stefan (TUD), Christoph Sprenger (KWB), Michael Rustler (KWB), Robert Schlick (TUD), Ralf Junghanns (TUD)

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Short summary

This report describes the first part of the SMART-Control web-based tool T1: "Initial risk assessment. Part A. Estimation of groundwater hydraulic residence time". The tool enables water utilities to estimate the groundwater hydraulic residence time at MAR sites by using temperature measurements in influent and recovered water. The tool was developed as collaboration between the project partners KWB (R code development) and TUD (web-based frontend implementation).

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ABSTRACT

Subsurface travel time from the area of recharge to the point of abstraction during MAR is a critical parameter to ensure sufficient attenuation for hygienic parameters and other undesired substances. A new simulation tool has been developed by the SMART-Control project partners KWB and TUD for determination of groundwater hydraulic residence time (HRT) using seasonal temperature fluctuations observed in recharge water and MAR recovery wells. This tool represents a proxy for quick, costs-effective and reliable control of travel time during aquifer passage. Time series of seasonal temperature measurements observed in surface water and abstraction wells can be fitted to sinusoidal functions. Peak values represented as local maxima and local minima and turning points from the fitted sinusoidal curves are used for the approximation of travel times between surface water and abstraction well. The calculated values are adjusted by a thermal retardation factor. The developed tool is user-friendly and offers the possibility to use existing hystorical temperature measurements as well as online sensor data. Data acquisition is resolved through the internal connectivity with other web-tools developed within the SMART-Control project, providing thus an integrated simulation environment.

CONTENT

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1. INTRODUCTION

1.1 MOTIVATION

The removal of pathogens from groundwater during subsurface passage represents a key component for the assessment of risks associated with managed aquifer recharge (MAR) sites (Sprenger et al., 2020). This is of crucial importance especially for riverbank filtration schemes where the recovered water is delivered to municipal supply systems as potable water. Luckily, microbial pathogens such as bacteria, protozoa and viruses are effectively removed from groundwater by complex decay mechanisms. The removal efficiency is influenced by site-specific conditions, with the degradation performance increasing together with the time spent in the subsurface. The groundwater hydraulic residence time (HRT) represents therefore an important indicator for the assessment of human health risks associated with groundwater recharge. Nevertheless, considering the diversity of microbial species, the aquifer heterogeneity and the variability of climate and operational conditions, it is not possible to predict an exact HRT needed to ensure the safe use of recovered water. Therefore, in compliance with national regulations, the operators of MAR facilities need to guarantee a minimum groundwater HRT that is generally considered sufficient for the natural removal of pathogens. This varies from country to country (i.e. 50 days in Germany) and depends on the characteristics of the aquifer and climate conditions.

1.2 SMART-CONTROL APPROACH

Different approaches are used for the estimation of mean HRT, including isotope analysis, numerical modelling, etc. These techniques are usually cost-intensive and cannot provide a real-time estimation of groundwater HRT at each recovery well of the MAR scheme. The main objective of SMART-Control is therefore to develop an innovative software tool for quick assessment and reliable characterisation of risks associated with MAR sites. The concept relies on two components: a sensor-based in-situ monitoring system for data acquisition and transfer, and a web-based simulation platform for data processing and simulations. The SMART-Control simulation platform is based on the openly accessible groundwater modelling platform developed by the Research Group INOWAS at Technische Universität Dresden, Germany. The platform contains a collection of empirical, analytical and numerical tools for assessing groundwater flow processes with focus on managed aquifer recharge applications (https://www.inowas.com). The INOWAS platform will be amended in the SMART-Control project by four additional simulation tools (Table 1). More info and the complete documentation of the tools is available at: https://www.smart-control.inowas.com/tools).

Table 1. Short description of simulation tools developed in the SMART-Control project

No.	Tool name	Tool description
T1	**Initial risk assessment**	The tool represents an easy-to-use instrument to evaluate the viability of a MAR project and the preliminary assessment of human health and environmental risks. The tool has two parts: A) a component for the estimation of groundwater hydraulic residence times during subsurface passage; and b) a component for quantitative microbial risk assessment (QMRA) of MAR schemes, including hazard identification, exposure assessment, dose analysis and risks characterisation. The risk will be assessed for selected reference pathogens such as bacterial, protozoan and viral pathogens for different hydraulic residence times during MAR.
T2	**Real-time monitoring and control**	This tool aims to facilitate the operational management of MAR sites. The tool includes a web-based monitoring system developed for real-time integration of time series data into the INOWAS modelling platform. Sensors installed at MAR facilities worldwide can be connected to the INOWAS platform to transfer collected data in real time. The data can be visualized, processed, downloaded and prepared for further usage.

No.	Tool name	Tool description
T3	**Automatic groundwater simulations**	Real-time observations collected from MAR sites will be integrated into a web-based modelling workflow. The system relies on existing groundwater modelling capabilities of the INOWAS platform, which will be expanded by adding additional features. The integration of real-time monitoring data into the simulation workflow will enable fast response time and optimized management, which helps to minimize and control the associated risks.
T4	**Predictions for advanced system management**	The tool will allow building climate change and development scenarios in the groundwater flow models to predict future boundary conditions and compare them to the present situation using the INOWAS Scenario Analyser. This will provide a novel way of using real-time, web-based groundwater models to assess the effects of climate change urbanisation, land use change (irrigation demand) and population growth on spatial and temporal water availability.

This report describes the main functionalities of the new tool **"T1. Initial risk assessment. Part A. Estimation of groundwater hydraulic residence time"**. For the description of the other tools see the project website: https://www.smart-control.inowas.com.

2. THEORETICAL BACKGROUND

The scientific background of the tool is rooted in the hypothesis that seasonal temperature variations in surface waters and abstraction wells can be used as potential tracers to estimate the groundwater hydraulic residence time during subsurface passage. At MAR sites, the groundwater temperature is directly influenced by seasonal temperature variations in the influent surface water. Under ideal conditions, these variations underlay a sinusoidal curve, with maximum values achieved in summer and lowest in winter. Under real conditions however, the approach needs to take into account also the retardation of heat transport in the subsurface due to multiple physical and site-specific factors. Thus, the real groundwater transport velocity is faster than the pore water velocity, leading to groundwater flowing faster than the temperature front propagation and the need of a correction factor accounting for this thermal retardation.

The mathematical concept of the tool consists in using a non-linear regression for fitting a sinusoidal curve to time series of temperature measurements taken at the points of recharge and extraction. To obtain plausible results it is necessary to select a full sine curve at both the inflow (surface water) and the outflow (groundwater), corresponding usually to a complete one-year cycle. After data selection, the measured temperatures are fitted for each full sine period separately to the general sinusoidal form according to:

$$f(x) = y_0 + \mathrm{A} \times \sin\left(\pi \frac{(x - x_c)}{w}\right) \qquad (1)$$

where:
y_0 = vertical shift or off-set
A = amplitude
x_c = horizontal shift or phase shift
w = period

This non-linear fitting is an iterative process carried out until convergence is reached. The fitted sine curve is then used to identify the dates of the peak values (local minima and maxima) and turning points (Figure 1). The time difference of the extrema between basin (surface water) and well (groundwater) results in a time offset that corresponds to the groundwater hydraulic residence time. However, heat is transported not only by the flowing water (convective heat flow), but also by heat exchange through solids and fluids (conductive heat flow). The mutual heat exchange of groundwater with the surrounding aquifer material retains the heat signal compared to pure advective transport, resulting in attenuation and retardation of the temperature signal along the flow path.

Calculated lag times between peak values and turning points in the basin and corresponding peak values in the groundwater need to be therefore corrected by a thermal retardation factor.

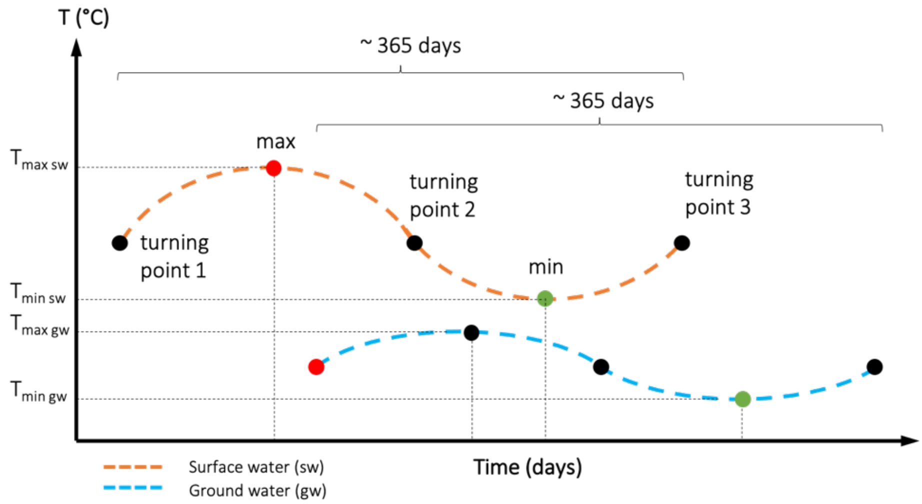


Figure 1. Calculation of min/max and turning points from the sine curve fitted to measured surface water (sw) and groundwater (gw) temperature data

To demonstrate the usability of temperature transport for the estimation of groundwater HRT, the project partner KWB tested this concept at the MAR site in Berlin in the framework of a previous research project (Sprenger, 2018). An algorithm was developed by KWB for fitting a full sinusoidal curve to seasonal data sets of temperature measurements in both infiltration ponds and recovery wells of the MAR facility.

The algorithm was developed in *R* language and is currently available on the GitHub repository at https://github.com/KWB-R/kwb.heatsine. One of the objectives of the SMART-Control project is to develop a web-based interface for this tool in order to facilitate the use of the code for assessing the groundwater residence time at MAR case studies. The web-based implementation of the tool includes three components that are described in detail in the next sections.

i. acquisition and integration of temperature measurements data (sub-chapter 3.1);
ii. processing of uploaded temperature time series (sub-chapter 3.2);
iii. calculation of groundwater residence times and results visualisation (chapter 4).

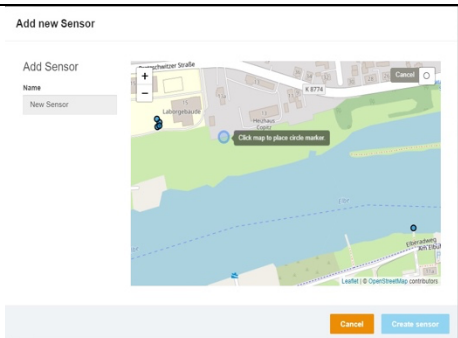
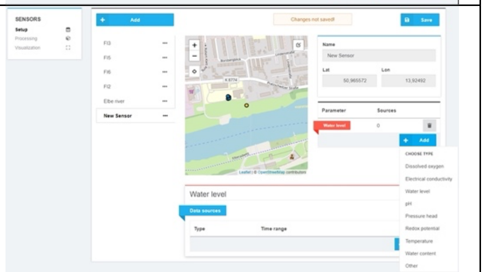
3. DATA ACQUISITION AND PROCESSING

The first two steps consist in uploading and processing of two temperature time series, one collected from the surface water that is used for infiltration and one from groundwater at the point of extraction. For this, the existing functionalities of the SMART-Control tool “Real-time monitoring tool” will be used. The tool is available on the SMART-Control simulation platform under the code T10 (online documentation available at https://inowas.com/tools/t10-real-time-monitoring/).

3.1 IMPORTING TEMPERATURE MEASUREMENTS DATA

The next paragraphs provide only a brief description of the required steps for data import and processing (Table 2). For a complete documentation of tool T10 see Deliverable D4.2 (Glass et al., 2020) and the online tool documentation.

Table 2. Brief description of main steps required for importing and integration of temperature measurement data using the additional SMART-Control tool "Real-time monitoring"

Step	Short description	Screenshot
Add observation point	Create a new simulation in T10 and add a new geo-referenced observation point of temperature measurements using the "+Add new sensor" button. The location needs to be included by clicking the specific location on the map. The exact geographical coordinates (WGS84) can be later updated. Note that location doesn't necessarily have to be associated with an online sensor, in this case it can be a manual or automatic monitoring station.	
Add parameter	For the created location, add parameter "temperature" by selecting "Add temperature" from the list of parameters. Note that other parameters can be associated with the observation point created, either by selecting them from the list or by adding new ones.	
Add data sources	To assign the source of temperature measurements, click on the parameter name and a new field will be created under the list of parameters. Time series data can be added by clicking the "+Add" button in "Data sources". Data can be uploaded as: • "*file*" (manual upload of CSV file), • "*online*" (from a FTP sensor connected to the INOWAS platform) or • imported from external web services using "*Prometheus*", an open-source interface for integration of online monitoring data. See online documentation of tool T10 for further detailed instructions about data import options. Note that multiple time series can be uploaded and combinations of the methods above are possible (i.e. data uploaded manually can be merged with online sensor data into one single time series).	

3.2 DATA PROCESSING

3.2.1 Value processing and time discretization

The uploaded data can be processed for further use in the "Hydraulic residence time" tool (and also other simulation tools in the INOWAS platform). Processing is divided into *time processing* and *value processing* (Figure 2, check the T10 documentation for detailed instructions).

Value processing comprises all processing algorithms which directly influence the values of a time series and includes mathematical operations as well as filtering rules. This can be used for example to exclude outliers, calibrate sensor data, etc. In the time processing section, gaps in the time series can be filled (interpolated) and the data set can be resampled to a different time resolution. For this, the interpolation method and the time resolution (Rule) needs to be defined. Note that the tool requires daily average temperature values so these features can be used to modify the time discretization i.e. from minutes, hours etc. into days.

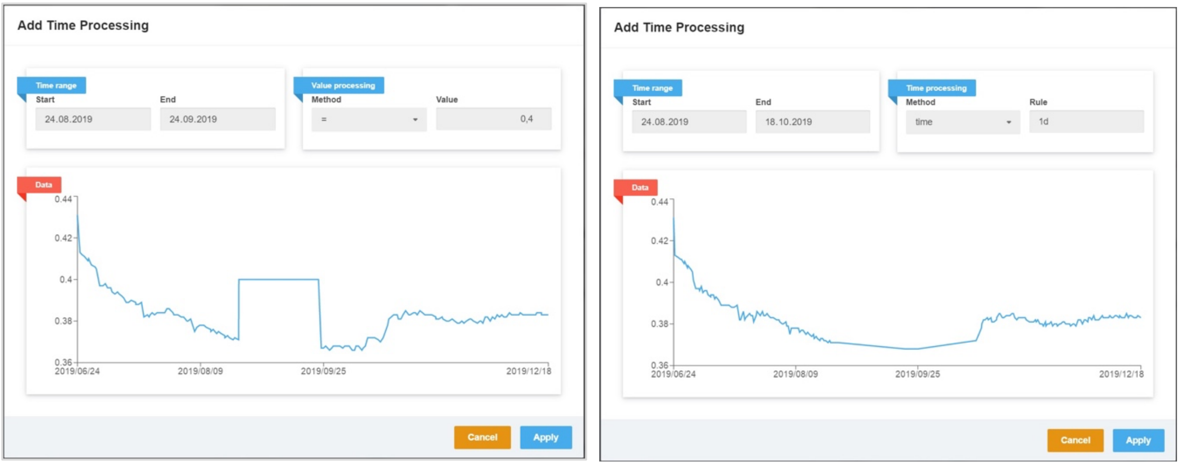


Figure 2. Data processing functionalities: value processing (left) and time discretization (right)

3.2.2 Time series "cropping"

For the calculation of groundwater HRT, the tool requires a time series of about one year. For this, use the "Cut" function in the time processing window to select a time range of about 365 days (Figure 3). Three processing rules are available: a) crop specific time period, b) crop from specified date until current day, and c) crop a specified number of units until current day. If the time series uploaded contains data from several years, try to select the year that is most representative and for which the seasonal variations can be described best by a sinusoidal curve.

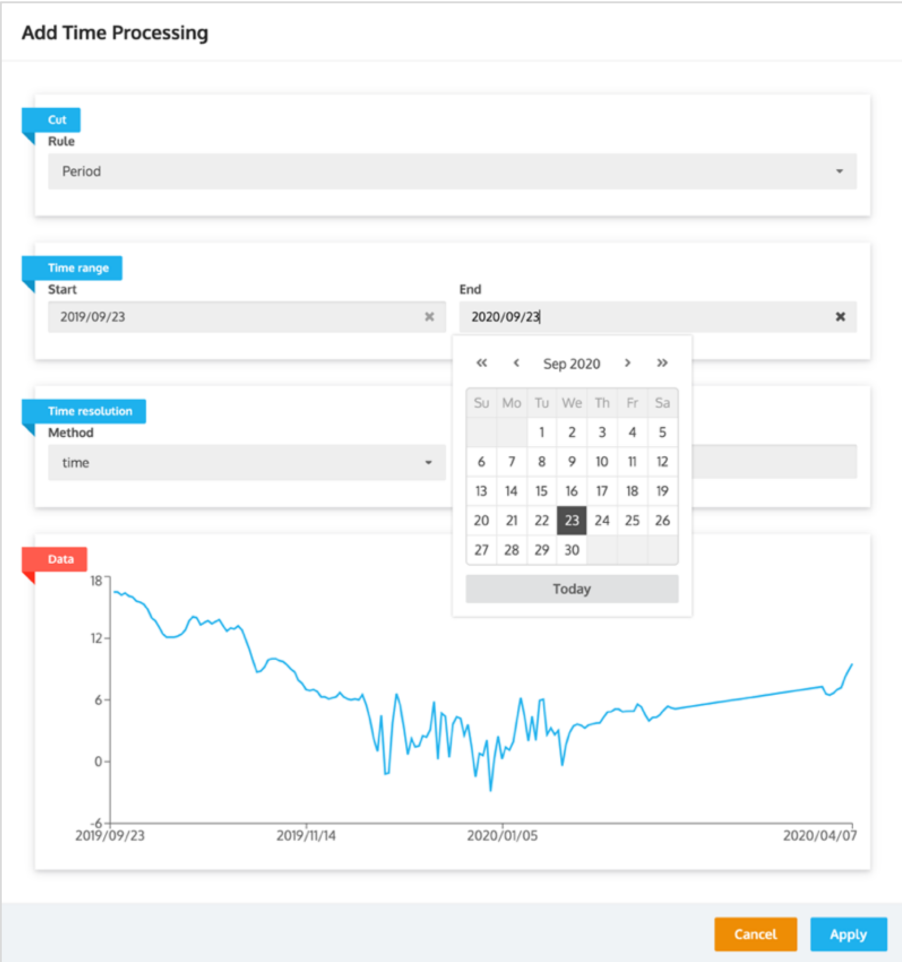


Figure 3. **Selecting a time range of one year during the time processing step**

The steps above can be repeated for importing and integration of further time series.

4. CALCULATION AND RESULTS VISUALISATION

To calculate the groundwater residence time using temperature time series uploaded in previous steps, open the tool T19 "Groundwater residence time" and create a new simulation. In the opening window, select the file with time series corresponding to surface water and groundwater temperature from the list of T10 instances. Note that the list contains all public instances of T10, including those created by other users. After choosing the instance, select the observation point ("sensor") for both inflow and outflow (Figure 4). In the example below, both time series have been prepared in T10 by selecting time range values between 23.04.2016 – 30.05.2017 for surface water and 19.06.2016 – 29.06.2017 (for groundwater), each interval representing approximately one year.

By default, a thermal retardation factor of 1.8 is considered, which corresponds to a sandy aquifer. The value can be edited, then the calculation can be started by clicking the button "Run calculation and save".

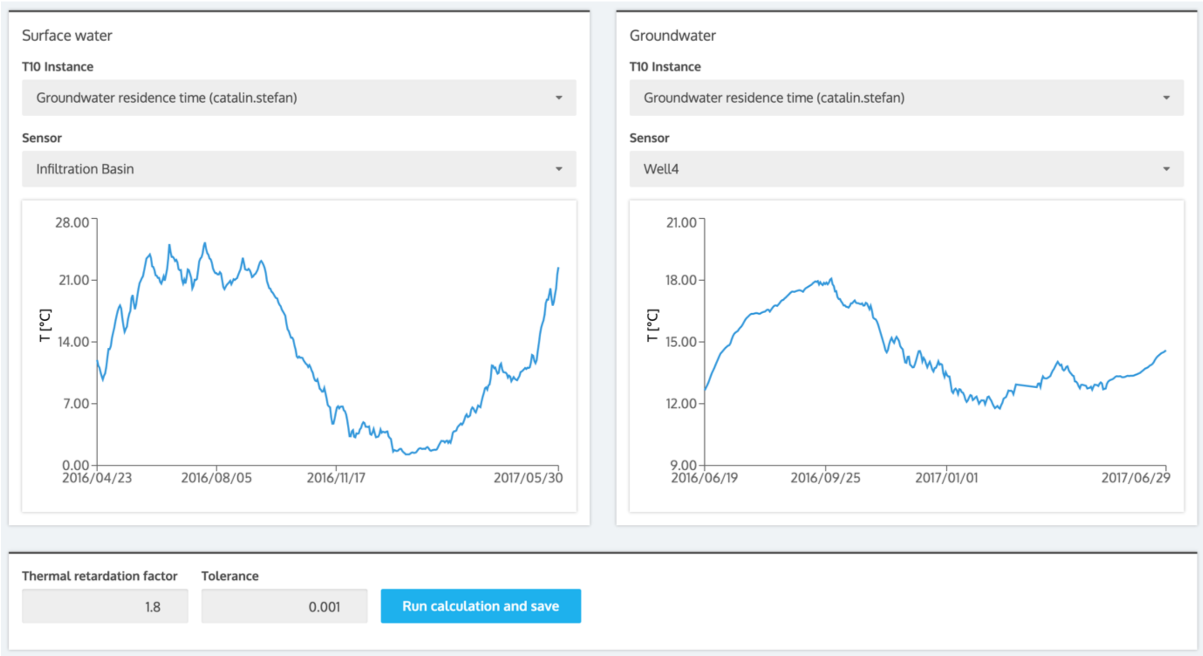


Figure 4. **Selecting the data sources for surface water and groundwater temperature time series.**

The results of the calculation are shown in Figure 5. The sine curve (blue line) is fitted to the temperature measurements (red line) and the max/min and observation points are displayed on the graphs. To facilitate visualisation and comparison, both graphs can be displayed using the same time scale (which emphasizes the time shift between temperature measurements in inflow/outflow) or by adjusting the time scale (in which case the curves are superimposed).

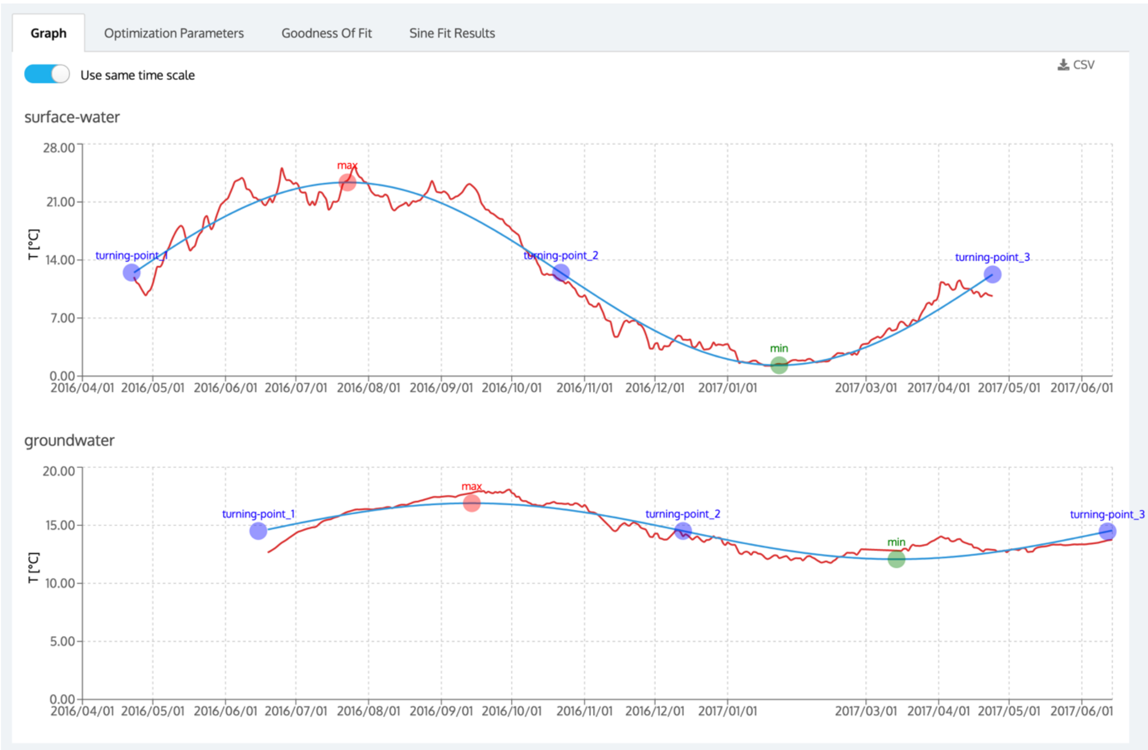


Figure 5. **Calculation results: graphic visualisation of sine curve fitting with display of calculated min/max and turning points for surface water and groundwater time series**

The other three tabs in the results section show the optimization parameters of the sinusoidal regression curve (see Eq. 1), the goodness of fit to the measured temperature data and, in the last tab, the times corresponding to the calculated max and min temperatures and the three turning points, as well as the calculated groundwater residence time with and without consideration of the retardation factor (thermal / hydraulic) (Figure 6). Each result can be then downloaded as CSV file.

Graph | **Optimization Parameters** | Goodness Of Fit | Sine Fit Results

CSV

	Surface Water (IN)	Groundwater (OUT)
period_length	367	362
alpha	11	2
beta	0	0
y0	12	14
a	11	2
x0	0	0

Graph | Optimization Parameters | **Goodness Of Fit** | Sine Fit Results

CSV

	Surface Water (IN)	Groundwater (OUT)
RMSE	1.5700	0.7100
R2	0.9600	0.8500

Graph | Optimization Parameters | Goodness Of Fit | **Sine Fit Results**

CSV

	Surface Water (IN)	Groundwater (OUT)	Residence Time [d]	
			Thermal	Hydraulic
turning-point_1	2016-04-22	2016-06-15	54	30
max	2016-07-23	2016-09-14	53	29
turning-point_2	2016-10-22	2016-12-13	52	29
min	2017-01-23	2017-03-14	50	28
turning-point_3	2017-04-24	2017-06-12	49	27

Figure 6. Calculation results: display of optimisation parameters of the sinusoidal regression curve, model's goodness of fit to the measured data and the calculated max/min and turning points for the two temperature time series

5. CONCLUSIONS

Subsurface travel time from the area of recharge to the point of abstraction during MAR is a critical parameter to ensure sufficient attenuation for hygienic parameters and other undesired substances. The simulation tool developed by KWB and implemented by TUD on the web-based INOWAS platform uses seasonal temperature fluctuations observed in recharge water and MAR recovery wells as a proxy for cheap and reliable control of travel time during aquifer passage. Time series of seasonal temperature measurements observed in surface water and abstraction well can be fitted to sinusoidal functions. Peak values represented as local maxima and local minima and turning points from the fitted sinusoidal curves are used for the approximation of travel times between surface water and abstraction well. The calculated values are adjusted by a thermal retardation factor.

The developed tool is user-friendly and offers the possibility to use existing hystorical temperature measurements and online sensor data. Data acquisition is resolved through the internal connectivity with other web-tools, providing thus an integrated simulation environment. In further developments, the possibility to provide automatic calculations of groundwater residence times will be explored, amended with functionalities for user notification when the calculated values drop below fixed thresholds.

6. REFERENCES

1. Glass, J., Junghanns, R., Schlick, R., Stefan, C. (2020) Implementation of web-based real-time monitoring tool on INOWAS platform. SMART-Control Deliverable 4.2 (available at http://smart-control.inowas.com/wp-content/uploads/2020/06/SMART_Control_D4_2.pdf).
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