The use of modelling to assess the interaction of surface water and groundwater in the area of Sihoť in Bratislava

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Abstract: The assessment of groundwater and surface water interactions is a current topic, because research of the issue can contribute to a better understanding of the dynamics of the natural environment. Numerical modelling is a suitable tool for solving surface and groundwater interactions. Through modelling, it is possible to simulate the ongoing processes in the area under study and create a hydraulic and heat transport model. The Sihoť Water Source was chosen as the area of study because it is an anthropogenically unaffected locality. During the compilation of the model and later in the calibration process, data on the temperature and level of the groundwater table and Danube water were used, which were available thanks to the monitoring that took place at the site. In the calibration process, the sensitivity of the parameters determined by calibration was also examined. During calibration and sensitivity analysis, the hydraulic conductivity was further investigated using so-called pilot points that had been entered into the model. The accuracy of the model was verified by automatic calibration using the PEST program, while the average error value was 0.21 m for the hydraulic model and 1.04 °C for the transport model. The knowledge and methodological procedures gained by examining the issue can be applied in many other cases, such as water quality analysis, assessment of the vulnerability of the groundwater and surface water regime, or in assessing the impact of extreme precipitation and other factors.

Key words: Surface and groundwater interaction, temperature, groundwater table level depth, modelling, transport and hydraulic model.

1. INTRODUCTION

Groundwater and surface water are two separate entities; however, they are undisputedly interconnected. The chemical, biological and physical properties of surface waters and groundwater are certainly very different and their interaction results in processes that lead to the transport, degradation, transformation, precipitation, or sorption of the substances contained in them. The interaction between groundwater and surface water has a major impact on the qualitative properties of energy, dissolved and insoluble substances, or organisms (Sophocleuos, 2002; Fleckenstein et al., 2010). The extent of interactions depends on the geomorphological, geological, hydrogeological, or climatic conditions of the area. The water exchange between the individual systems depends not only on natural factors, but also on anthropogenic ones. Anthropogenic activity can have a negative impact on exchange processes, which can lead to toxic and organic contamination with an adverse environmental impact (Fľaková et al., 2020). The development of groundwater temperature with anthropogenic influence in the region of Bratislava has previously been examined by Krčmář et al. (2020) and Hodasová et al. (2020). In the case of surface and groundwater interactions, the chemical composition of one system or another is affected, depending on the suitability for public water supply, as well as the ecological status of surface waters (Palmer et al., 1992; Sophocleuos, 2002).

The first numerical models developed for the given scientific problem were created in the 1980s and simulated the processes of water exchange between groundwater and surface water. Due to technical limitations, these models were greatly simplified and modelled as homogeneous units (Prudic, 1989). In the following period, one can observe the effort to develop more complex, integrated models of surface-subsurface components of the hydrological system. Since the 1990s, various research activities have taken place in the given sphere, increasingly linking disciplines from hydrology and hydrogeology to ecology, biogeochemistry, and environmental studies (Krause et al., 2009). At the turn of the century, scientific interest in the issue increased, which was conditioned by the adoption of new legislation, such as the EU Water Framework Directive (Krause et al., 2009; Fleckenstein et al., 2010). In the last two decades, research on surface and groundwater interactions has received increasing attention. Several studies have been published that provide insight into new assessment methods and approaches. Increased interest in this issue is based on the efforts to introduce new approaches to monitoring and modelling, as well as effective and integrated management of water resources (Ebrahim et al., 2013). A summary of the basic concepts of groundwater and surface water interactions from a predominantly hydraulic-hydrogeological point of view is contained in Sophocleous (2002). Anibas et al. (2012) present specific types of surface and groundwater interactions, as well as regional modelling approaches. The evolution of surface and groundwater interactions in relation to climate change has previously been discussed by Guevara-Ochoa et al. (2020), Scibek et al. (2007), and Saha et al. (2017). Case studies of surface and groundwater interactions have also been the subject of research in Slovakia, namely by Krčmář (2012), Dušek & Velísková (2017), and Krčmář et al. (2018).

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Dušek & Velískova (2015) dealt with the quantification of surface and groundwater interactions on the territory of Žitný Ostrov, to which they applied numerical modelling in the MODFLOW program. Output data of one-dimensional numerical modelling of surface water in a river were used as input data for a three-dimensional numerical simulation of groundwater flow. The solution of temporal and spatial variability at the interface of the surface water and groundwater is crucial for determining the dynamics of the chemical composition of an aquifer. Keery et al. (2007) addressed the temporal and spatial variability of groundwater and surface water flow in Stoke on Tern, England. Passadore et al. (2015) dealt with the characterization of temporal and spatial variability of the groundwater and surface water interactions on the example of the river Brenta (Veneto, Italy). Saha et al. (2017) in their case study on the Kiskatinaw River in Canada evaluated the temporal dynamics of the interaction of groundwater and surface water due to the impact of climate change. The results confirmed that climate change significantly affects the course of the interaction between the surface and groundwater. Stefania et al. (2018) evaluated the impact of groundwater exploitation on surface water resources in the Aosta Plain Alpine Valley in north-western Italy using the MODFLOW – 2005 program. Anibas et al. (2009) applied vertical temperature profiles to quantify the interaction of the surface and groundwater. Temperature time series were monitored for over a year at several depths below the river bottom in Belgium, as well as in lake sediments in East Germany. Vertical temperature profiles were also supplemented by analytical solutions for steady flow and one-dimensional heat transfer. In conclusion, the use of a simple analytical solution for vertical heat transfer with temperature data observed at preselected depths provides a cheap and simple method for obtaining information on the direction of exchange between the groundwater and surface water. Rau et al. (2010) used heat as a natural indicator of the interaction of surface and groundwater in Maules Creek in New South Wales in Australia.

The aim of the study is to evaluate the interaction of surface and groundwater in the Sihoť area in Bratislava using modeling tools. For this purpose data obtained through monitoring at the site were used. The evaluation was based on a compilation consisting of a hydraulic and a tranport model in the MODFLOW-USG programme. Deeper analysis of input parameters were analyzed using automatic calibration PEST and by pilot points.

2. STUDY AREA

The Sihoť water source is situated in the south-western part of Slovakia, in the Karlova Ves district of Bratislava. The investigated area is located on the Sihoť (Danube Island) and is bordered by the Danube River and the Karlova Ves river branch (Fig. 1; Varga & Panák, 2018; Water Museum, 2021).

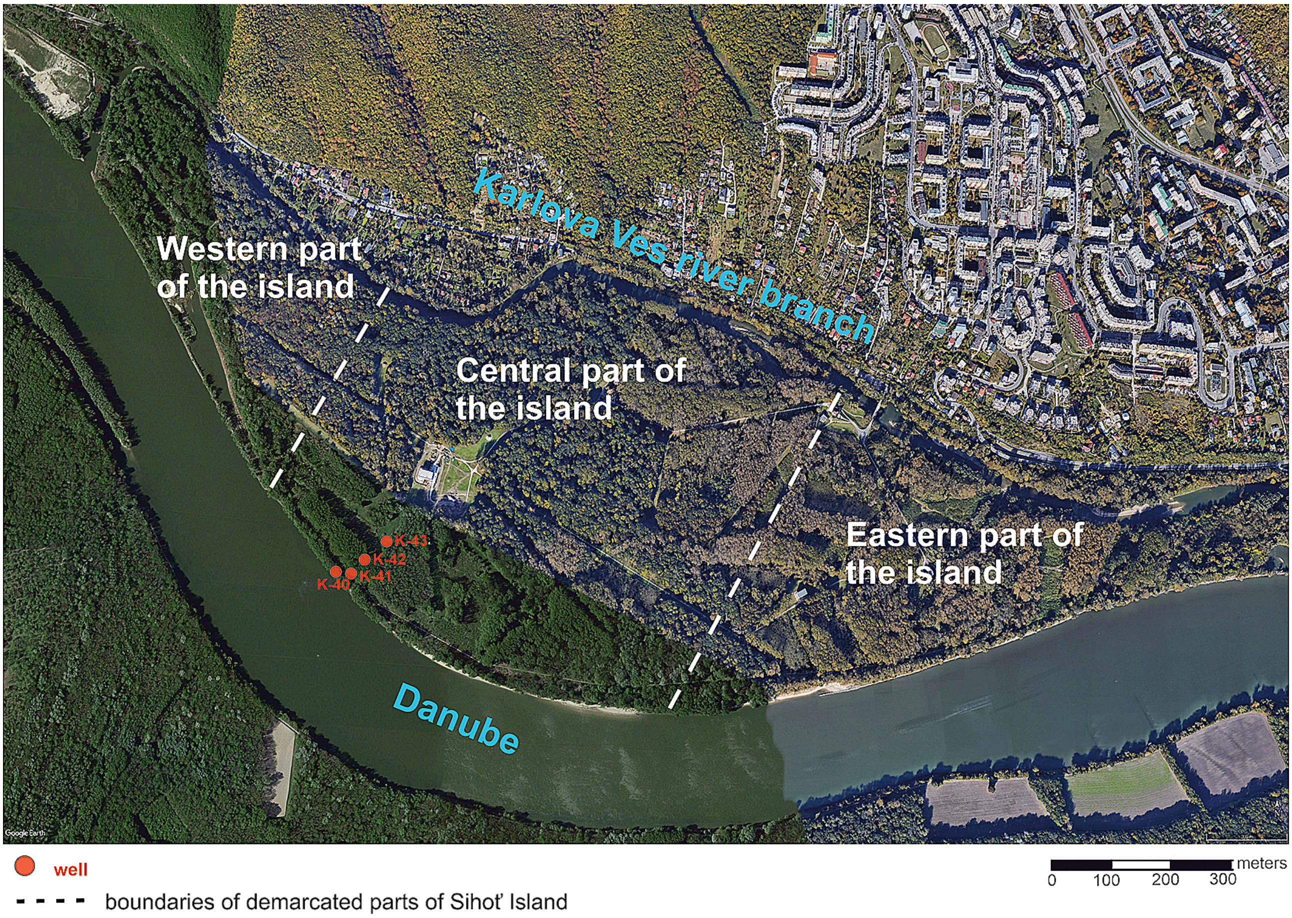


Fig. 1. Location of area of interest (modified according to Google Earth, 2021) and situation of monitoring wells

In accordance with the regional geomorphological division of Slovakia according to Mazúr and Lukniš (1986) the studied area is located at the junction of two areas – The Fatra-Tatra and Danubian Lowland. Within the Danubian Lowland, the landscape of the Danube Plain is present; the rest of the area is surrounded by the mountain landscape of the Little Carpathians. The terrain of the Sihoť area ranges from 137 to 138 m above sea level.

Based on the climatic zoning of Slovakia, the investigated area belongs to a warm area, which is characterized as warm, slightly dry, with a mild winter (Lapin et al., 2002 in The Landscape Atlas of the Slovak Republic, 2002). Based on the Map of Climate Geographical Types (Kočický & Ivanič, 2011), the Sihoť area belongs to the climatic-geographical type with a lowland climate.

The geological structure of the study area consists of Paleozoic, Neogene and Quartenary sediments. The Palaeozoic sediments in the investigated area are represented mainly by granitoid rocks – granites, granodiorites and diorites. Neogene sediments are represented by coarse-grained sands, fine gravels, cemented calcareous sands, clayey sands and clays. Quaternary sediments are represented in the area mainly by fluvial alluvium of the Danube - gravel accumulations present in the terraces and Holocene sand-silt cover. Fluvial-organic sediments, as well as clayey humus-rich clays are present in the places of the Karlova Ves river branch. Redeposited alluvial sandy gravels of the riparian zone are also present in small quantities on the island of Sihoť (Žák & Kovács, 2009; Polák et al., 2011).

Groundwater in the investigated area is concentrated in the gravelly sediments of the fluvial alluvium of the Danube River. They represent a bedded collector with intergranular permeability and have vertical and horizontal variability in particle size distribution, permeability and geometric properties (Varga et al., 2010). In the horizontal direction, the aquifer is delimited from the north by Palaeozoic rocks, which are sunken due to the fault zone located near the bypassing branch of the Karlova Ves river. Palaeozoic rocks are present in the subsoil of Quaternary fluvial sediments as well as in the subsoil of Neogene sediments. The boundary of the aquifer on the southern side is formed by the river Danube. In the vertical direction, relatively permeable and semi-permeable sediments, such as sands and silty sands, are relatively permeable in the overburden of the aquifer. The subsoil of the aquifer is formed by the Neogene sediments and Palaeozoic rocks. The aquifer is heterogeneous and anisotropic. Sand-silty gravels, sandy gravels or gravels with an admixture of sand alternate. The aquifers have the highest thickness in the central part of the territory. The thickness decreases towards the west and east side (Benková et al., 2005; Benková et al., 2013).

The hydraulic conductivity is in the order of magnitude 10^{-2} to 10^{-3} m·s^{-1}. Gravel-sandy sediments in the given area are characterized by high permeability and high transmissivity (Žák & Kovács, 2009; Varga et al., 2010). The primary regime factor that affects the qualitative-quantitative regime of groundwater is the Danube River. The Danube River directly affects the change in the amount of groundwater, the operating regime of the use of individual wells and the quality of the groundwater withdrawn. A close hydraulic connection is applied between groundwater and surface water in a given area. This hydraulic connection is especially present between the level of the river Danube and groundwater. However, it is present to a lesser extent between the groundwater and surface water in the Karlova Ves river branch (Pospíšil et al., 1999).

The quality of the groundwater in the territory of Bratislava is diverse and depends on the degree of anthropogenic activity in the given area, as well as on the ongoing physico-chemical processes, such as the influence of deep CO_2 or fluctuations in the surface flow levels. The chemical composition of groundwater is also significantly influenced by the chemical composition of the surface water of the Danube, as well as the nature of the infiltration area and bottom sediments (Ženišová et al., 2000; Ženišová et al., 2018).

3. MATERIAL AND METHODS

3.1. Monitoring

Groundwater levels and groundwater temperatures were monitored in the Sihoť area as part of monitoring in wells K-40, K-41, K-42 and K-43. Monitoring took place from 2015 to 2019. The location of the wells within the island of Sihoť is shown in Fig. 1. The depth of the wells is given in Tab. 1. Measurements were performed automatically using Solinst data loggers (model Levelloger Junior Edge 3301). Groundwater levels and temperatures were recorded at hourly intervals, and the data were transferred to a computer via an optical reader.

Tab. 1. Depth and altitude of monitoring wells in the Sihoť area

Well designation	Altitude Well casing [m a. s. l.]	depth [m]
K-40	139.27	10
K-41	139.16	10
K-42	138.64	10
K-43	139.24	10

3.2. Modelling

The MODFLOW-USG program, which is implemented in the Groundwater Vistas program, was used to build the hydraulic and transport model. MODFLOW-USG simulates groundwater flow using a generalized control volume finite-difference approach. MODFLOW-USG implements a transport model called the Block-Centered Transport (BCT) Process for MODFLOW-USG (Panday, 2020). One of the first steps in compiling the model was to choose the appropriate spatial and temporal discretization of the environment. In spatial discretization, the researched environment was represented by a model grid consisting of columns, rows, and layers. The geological structure of the area was taken into account by the vertical division of the area into layers. In the case of time discretization, the total simulation time was divided into time periods in which the change in the groundwater level and temperature was addressed. The constant values of the dependent variables were defined by the length of the time period (defined by the start and end numbers of the time period; Anderson et al., 2015).

The creation of a hydraulic and transport model was based on the definition of temperature and hydraulic parameters of the environment. The values of these parameters were initially estimated on the basis of the available literature, where values were found for a similar type of aquifer. Subsequently, these parameter values were adjusted based on monitoring data during the calibration process. The next step in developing the model was to define the boundary conditions. The time-varying Danube water levels were entered as boundary condition to the western side. This boundary condition was put in layers 14 – 17. The boundary condition 'Constant Head' was defined on the eastern side of the model for layers 15-21 and represented the average groundwater level. This was determined on the basis of data from the K-43 observation well. For the transport model, the conditions were defined as transient, i.e., the temperature changed over time. A Temperature boundary condition was specified for the entire area of the first layer. Using this boundary condition, the changing air temperature was set during the specified simulation time. On the western side of the model, a boundary condition was added, where the changing temperature of the Danube water was entered. The boundary condition was defined for layers 14 – 17.

3.3. Calibration

The process of calibration of the hydraulic and transport model can be defined as the modification or optimization of one or more input parameters of the model so that the values calculated by the model are as close as possible to the measured monitoring data. In the case of the investigated area, the method of automatic calibration using the PEST program was used. The PEST program is integrated into the Groundwater Vistas 8 program. There were two prerequisites for using PEST. The first was the import of so-called targets to the places where the measurements were performed. The second assumption was to define the parameters that will be subsequently estimated. In the case of the investigated area, the targets were wells (K-40 to K-43), in which the temperature and groundwater level were measured. They were entered into the model via Analytical Elements. The second assumption was to define the parameters that would be estimated when running PEST. In this step, a group of parameters was defined, with minimum and maximum allowed value. A logarithmic transformation of the parameters was also used. Once these prerequisites were met, the PEST could be started. During iteration, the model was run once or twice for each parameter.

As part of the automatic calibration using the PEST, it was possible to use the so-called pilot points. Through the pilot points, it was possible to determine the spatial distribution of the hydraulic conductivity. As in the case of the PEST, the hydraulic conductivity was not bound to the layers, but varied across the defined zones. The pilot points were entered into the model via analytical elements. They can be entered manually (e. g., at observation points) or automatically using the "Quick Pilot Points" function. In the case of a given function, it was necessary to define the distance between individual pilot points in the settings so that they sufficiently cover the research area. Furthermore, it was necessary to determine the range of values of the hydraulic conductivity; in this range, the value of the hydraulic conductivity was sought in place of the pilot points (Rumbaugh et al., 2020).

The values of the hydraulic conductivity, which were determined at the location of the pilot points were interpolated by means of the kriging method for the remaining points of the model grid. This is the most representative geostatistical method. The interpolation process using the kriging method requires a suitable variogram. The variogram is a three-dimensional function that is used to determine the spatial correlation of the observed model variables. (Sefelnasr, 2007; Kareem, 2018).

Upon completion of the calibration, the correlation between the measured and modelled results was determined. For this purpose, it was possible to use calibration statistics, which is available in the Groundwater Vistas 8 program. The quality of the calibration was determined on the basis of the error value, or residual values (Rumbaugh et al., 2020). The residual value is the difference between the measured and calculated groundwater levels or temperatures. The calibrated model should have the lowest possible residual value. A negative value indicates that the value of the parameter calculated by the model is higher than the value of the parameter measured within the monitoring. Conversely, a positive value means that the calculated value of the parameter is lower than the measured value. Another indicator is the residual mean, which is calculated by dividing the sum of the residuals by the number of residuals. The absolute residual mean defines the average error rate of the model. The sum of squared residuals indicator expresses the difference between the squares among the observed and calculated variables, and the root mean square error characterizes the degree of variance of residual values (Geotrans, 2005; Anderson et al., 2015; Kaarem, 2018).

4. RESULTS

4.1. Hydraulic and transport model

The model was built as a two-dimensional (in section) with computational grid divided into 1 row and 100 columns, which significantly simplified the model environment. The model was vertically divided into 23 layers, of which layers 1 – 10 represented the aeration zone, layers 11 – 21 the aquifer and layers 21 – 23 represented the impermeable Neogene subsoil. The Groundwater Vistas 8 program was used to compile it, and the MODFLOW-USG program was applied for the modelling itself. The input parameters that were entered for the calculation of the hydraulic and transport model are given in Tab. 2. The values of the hydraulic conductivity were defined for 3 zones. These corresponded to the vertical distribution of the layers based on the geological structure of the area. The model also addressed water flow and transport through the unsaturated zone. To solve the unsaturated zone, it was necessary to enter the parameters of Alpha, Beta, residual saturation, and the Brooks-Corey exponent into the model. These were then entered into Richards' equation with the van Genuchten function, which calculates moisture content retention, as well as the Brooks-Corey function, which calculates relative permeability. The Richards equation is implemented in MODFLOW-USG (Rumbaugh et al., 2020). The hydraulic and transport model was built for transient flow conditions. This means that the groundwater depth and water temperature have changed over time. The length of time step was 1 month and the total simulation period was set at 60 months (period 2015–2019).

Tab. 2. **Input parameters for hydraulic and transport model determined according to Hecht-Mendéz (2008) and Panday (2020)**

	Hydraulic parameters	value
Zone 1	hydraulic conductivity $K_x = K_y$	$4 \cdot 10^{-8}$ m·s^{-1}
	hydraulic conductivity K_z	$1 \cdot 10^{-5}$ m·s^{-1}
Zone 2	hydraulic conductivity $K_x = K_y$	$5 \cdot 10^{-3}$m·s^{-1}
	hydraulic conductivity K_z	$5 \cdot 10^{-4}$ m·s^{-1}
Zone 3	hydraulic conductivity $K_x = K_y$	$6 \cdot 10^{-7}$ m·s^{-1}
	hydraulic conductivity K_z	$9 \cdot 10^{-7}$ m·s^{-1}
	porosity	0.35
	initial water table level	138 m a. s. l.
	rock matrix density	2630 kg·m^{-3}
	specific storage	0.01
	specific yield	0.25
Zone of aeration	Alfa	0.01
	Beta	5
	residual saturation	0.1
	Brooks-Corey exponent	3.5
	Transport parameters	
	longitudinal dispersivity	37.58 m
	transverse dispersivity	10 m
	transverse vertical dispersivity	2 m
	diffusion coefficient	2.5 m^2·s^{-1}
	distribution coefficient	$1.3 \cdot 10^{-4}$ m^3·kg^{-1}
	initial temperature	11.7 °C
	water thermal conductivity	0.65 W·m^{-1}·°C
	water thermal capacity	4174 J·kg^{-1}·°C
	density of water	1000 kg·m^{-3}

The heat transport model for the studied area was processed using the MODFLOW-USG program, using the BCT module. In the case of transport calculation, an initial temperature of 11.7 °C was entered into the model, which represents the average groundwater temperature. The heat transport model for the Sihoť area is shown in Fig. 2. Based on the transport model, it is possible to see the changing temperature in the area affected by the groundwater flow.

4.2. Calibration

The calibration of the model was performed in an automated way using the PEST program. The prerequisite for the use of the PEST was the import of observation objects and the determination of monitored parameters (Rumbaugh et al., 2020). There were 4 monitoring wells in the area, which provided information on the development of temperatures and groundwater depth with the help of installed data loggers. Monthly average values in probes

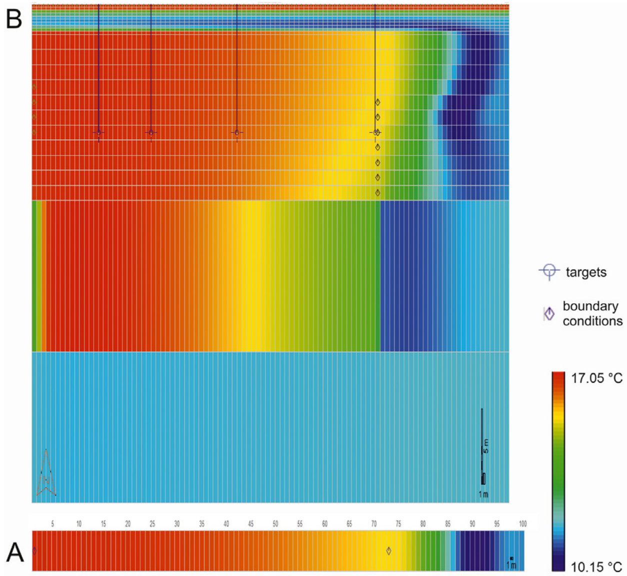


Fig. 2. **Heat transport model a. in plan view, b. in section**

K-40 to K-43 were calculated from the measured data. These were subsequently imported into the model as so-called observation objects through the function of analytical elements. After defining the observation objects, the parameters and range of their values were determined. After entering the required parameters, it was possible to start the PEST. The program then automatically changed the values of the calibrated parameters and performed a model solution. The values of the adjusted input parameters after calibration are given in Tab 3. From Tab. 3, it can be seen that the porosity parameter, the elastic storativity coefficient, and the longitudinal dispersivity were slightly changed, and the value of the distribution coefficient changed slightly as well. The values of the specific yield, unsaturated zone parameters (alpha, beta, residual saturation, Brooks-Corey exponent), and transverse dispersivity did not change during calibration.

Tab. 3. **Change of input parameter values after calibration**

	Hydraulic parameters	Input values	Change in values after calibration
	porosity	0.35	0.4
	specific storage	0.01	$5.5 \cdot 10^{-3}$
	specific yield	0.25	0.25
Zone of aeration	Alfa	0.01	$9.9 \cdot 10^{-3}$
	Beta	5	4.998
	residual saturation	0.1	0.1
	Brooks-Corey exponent	3.5	3.5
	Transport parameters		
	longitudinal dispersivity	37.58 m	29.33 m
	transverse dispersivity	10 m	10 m
	distribution coefficient	$1.3 \cdot 10^{-4}$ m^3·kg^{-1}	$1.89 \cdot 10^{-4}$ m^3·kg^{-1}

During the automatic PEST calibration, the possibility of entering the pilot points into the model was used (Fig. 3). Using them, the PEST program then calculated the value of the hydraulic conductivity for each cell of the model. However, this can only be done for layers in which there were also calibration points (points with measured data). Therefore, it was possible only for the layer that represented the aquifer. Only one value of the hydraulic conductivity was determined for the unsaturated zone and the underlying Neogene, which was valid for the whole layer. Changes in the values of the hydraulic conductivity, which were estimated using pilot points, can be found in Tab. 4.

The main goal of the calibration was to find out the agreement between the measured and modelled results. The quality of the overall calibration as well as the agreement between the measured and modelled results was determined using a set of statistical methods. Statistical indicators for the hydraulic and transport model can be found in Tab. 5. The overall quality of the calibration was indicated by the error value, or residuals value. The residuals values were calculated for each observation object. In the case of the hydraulic model, the value of the residual mean was equal to -0.21 m, and for the transport model, the residual mean was equal to 1.04 ° C.

Calibration was also evaluated using graphs. The first type is a scatter plot, where the measured values were plotted against the values calculated by the model. For an ideal calibration, the points should be close to a line with an inclination of 45 °, i.e., the calculated value is equal to the measured value. The degree of variance theoretically determines the degree of overall calibration quality (Rumbaugh et al., 2020). Fig. 4 displays the plot

Tab. 5. Calibration statistical indicators for calibrated hydraulic and transport model

Hydraulic model	Value [m]
Residual Mean	−0.21
Residual Standard Deviation	0.3
Absolute Residual Mean	0.29
Sum of Squared Residuals	2.00E+01
Root Mean Square Error	0.36
Minimum Residual	-0.95
Maximum Residual	0.72
Range of Observations	3.27
Transport model	**Value [°C]**
Residual Mean	1.04
Residual Standard Deviation	2.12
Absolute Residual Mean	1.95
Sum of Squared Residuals	1.08E + 03
Root mean Square Error	2.36
Minimum Residual	−4.04
Maximum Residual	5.26
Range of Observations	18.2
Number of Observations	193

Tab. 4. Changes in the values of estimated hydraulic conductivity using pilot points

	label of pilot points	value [m·s^{-1}]
zone 1	k_xP1	1.16·10^{-2}
	k_zP1	1.16·10^{-3}
zone 2	k_xP21	1.16·10^{-2}
	k_xP22	1.16·10^{-2}
	k_xP23	1.16·10^{-2}
	k_xP24	8.81·10^{-3}
	k_xP25	2.38·10^{-3}
	k_xP26	1.03·10^{-3}
	k_xP27	1.16·10^{-2}
	k_xP28	6.41·10^{-3}
	k_xP29	1.16·10^{-7}
	k_xP30	1.16·10^{-7}
	k_zP21	1.02·10^{-4}
	k_zP22	1.37·10^{-5}
	k_zP23	6.42·10^{-6}
	k_zP24	2.83·10^{-3}
	k_zP25	5.14·10^{-5}
	k_zP26	2.47·10^{-7}
	k_zP27	1.12·10^{-6}
	k_zP28	1.16·10^{-2}
	k_zP29	5.07·10^{-8}
	k_zP30	7.72·10^{-7}
zone 3	k_xP4	1.22·10^{-7}
	k_xP4	1.32·10^{-8}

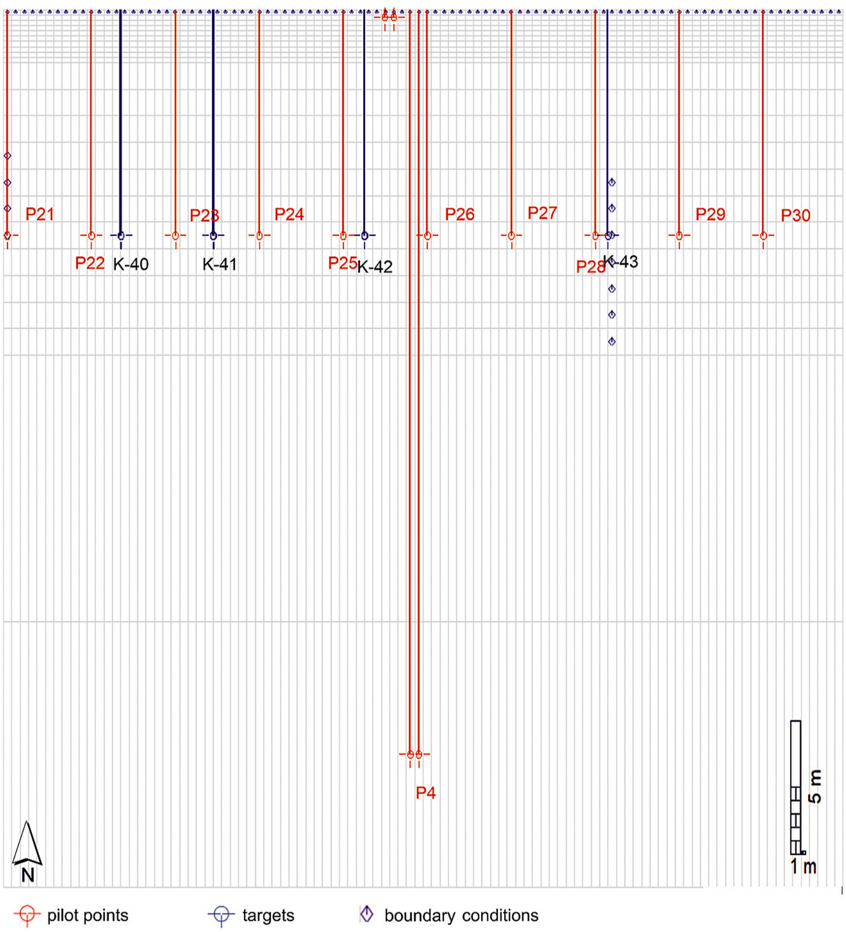


Fig. 3. Display of pilot points and observation objects within the determined model

Fig. 4. Display of measured and calculated groundwater levels

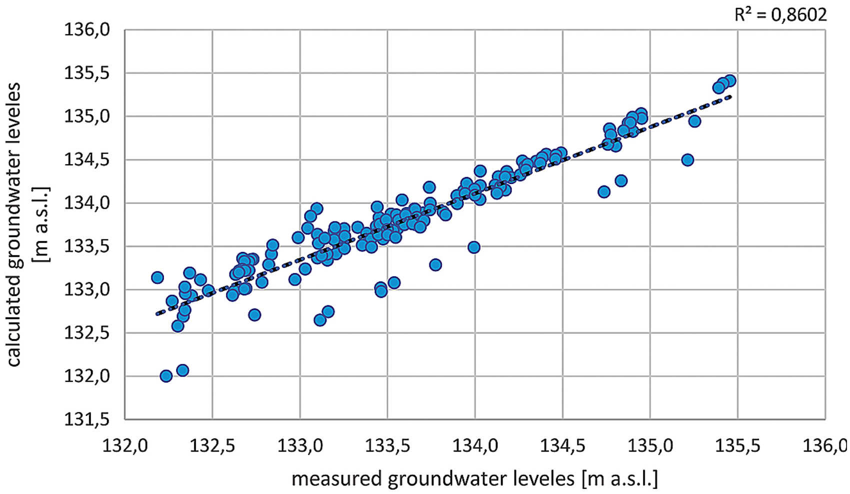
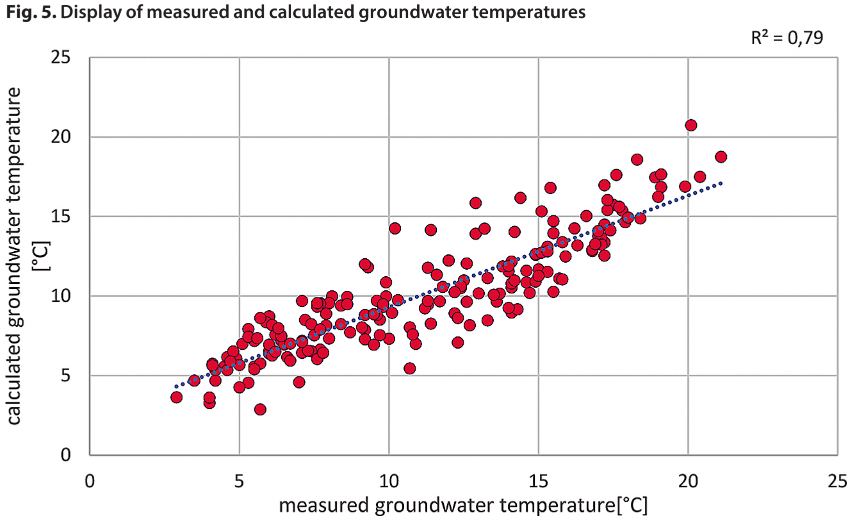


Fig. 5. Display of measured and calculated groundwater temperatures



of calculated and measured groundwater levels. It is evident that the degree of scattering was small and the calibration was successful. The degree of tightness according to the coefficient of determination R^2 was very high. The higher degree of scattering can be seen in Fig. 5, where the measured and calculated groundwater temperatures were plotted. Based on the coefficient of determination R^2, there was a high tightness between the observed and simulated temperatures. Even in this case, the calibration process seems to be successful enough.

5. DISCUSSION

5.1. Modelling

The issue was addressed using modelling in the Groundwater Vistas environment. The MODFLOW-USG program was used, which made it possible to directly solve heat transport in the BCT module. MODFLOW-USG for the heat transport model was developed in the work of Falakdin, 2019. Falakdin (2019) compared the results of the solution from the MODFLOW-USG environment and from the MODLOW-2005 environment using the MT3DMS module. The conclusion was that MODFLOW-USG provided a greater degree of flexibility in grid design. Due to the smaller number of cells, the calculation was faster.

For the transport model, an initial temperature of 11.7 °C was entered, which represented the average groundwater temperature. A boundary condition of varying air temperature was entered into the first layer. The second boundary condition was the changing average monthly temperature of the Danube water. The effect of air temperature was seen in the uppermost parts of the aeration zone. With increasing depth, the temperature fluctuation diminishes until it reached a constant value. Duque et al. (2010) also illustrated that temperature changes in the uppermost layers are in the air temperature range of 15–21 °C. According to Garcia-Gil et al. (2014), the fluctuation of the river level had a significant effect on the groundwater temperature up to a distance of 200–300 m. The maximum calculated temperature difference of 6 °C was recorded in winter, when the temperature of the infiltrating surface water was different from the temperature of the aquifer. Duque et al. (2010) showed that temperature changes reached a depth of 15 to 40 m and were related to a period of higher water flows in the river. In a study by Xie et al. (2017), it was reported that river temperature affects groundwater temperature to a depth of 9 meters of aquifer. In our case, we can see that the temperature of the Danube water manifested itself in the entire aquifer to a depth of 13 meters and also interfered with the underlying Neogene, where, however, it faded out rapidly (Fig. 2). However, the influence of surface temperature is also an important parameter, which fundamentally affects the groundwater temperature, and at a distance of several tens of meters to the hundreds of meters from the river, the influence of surface temperature begins to prevail over the influence of river temperature. Although heat transport is closely linked to groundwater flow, heat dissipation is also determined by other processes, namely: dispersion, diffusion or conduction. According to Molina-Giraldo et al. (2011) coefficients of dispersion are usually assumed to be dependent on the fluid velocity and particle size of the porous media. Park et al. (2015) pointed out that an increase of thermal dispersion occurs with an increase of flow velocity. The calibrated value of the longitudinal dispersion was 29.33 m. This higher value included both dispersion process and the heat dissipation due to regular surface water level fluctuations and surface water gradients. Transverse vertical dispersion had no effect in the model because the heat transfer to the other layers was caused by conduction. The solution of heat transport with a combination of level change leads to more exact solutions, especially at a distance of several meters from the river (Xie et al., 2017). The monitoring probes used in the study by Xie et al. (2017) were located at a distance of 100 m from the river. The modelling results showed that the river temperature no longer has any effect on the groundwater temperature at such a distance. The vertical heat transfer from the Earth's surface to the aeration zone was decisive. In our case, the K-43 probe was the furthest from the Danube River, namely 136.45 m. It can be seen that at this distance the temperature oscillations were damped and heat transfer from the terrain surface to the aeration zone takes place in particular.

5.2. Calibration

The model for the Sihoť area was calibrated in an automated way using the PEST program. Mbonimpa et al. (2015) compared automatic calibration using the PEST program with conventional manual calibration. They state that automatic calibration can overcome the weaknesses of manual calibration, particularly in the high subjectivity factor, but that there may be an overestimation of the values due to failure to take into account the specific conditions examined. The degree of correlation between the measured and modelled data was determined by means of calibration graphic outputs. In the case of the table level, the coefficient of determination was equal to 0.86. When displaying the measured versus calculated temperature, the coefficient of determination was lower and had a value of 0.79. In the study by Garca-Gil et al. (2014) on the river Ebro, calibration statistics showed linear regression (R^2) values equal to a level of 0.97 and a temperature of 0.92.

The pilot point approach evaluates parameters as a spatially variable distribution. Due to the high influence of the hydraulic conductivity on the accuracy of the solution, the pilot points were added to the model. Using this method, the estimation of the values of the hydraulic conductivity was not tied to the previously determined zones, but was calculated for each cell of the computational network within the whole model for all layers in which the observation points were present. Hydraulic conductivity values were interpolated from a set of points distributed within the model domain using geostatistical method – kriging. The degree of heterogeneity and the values of hydraulic conductivity were determined by set of points at particular locations. The result of the pilot point approach was smoother parameter distribution as compared to zone-based parameter assignment. The pilot point calibration approach is more flexible and robust in comparison to manual calibration techniques (Usman et al., 2018). Baalousha et al. (2019) showed that the number, location and configuration of the pilot points had a significant impact on the calibration process, especially in highly permeable areas corresponding to karst areas. Automatic calibration is an efficient tool, however, it is a time-consuming process that takes several hours.

6. CONCLUSION

The aim of the paper was to evaluate the interaction of groundwater and surface water in the Sihoť water source in Bratislava. The evaluation of the issue was based on modelling – the creation of a hydraulic and heat transport model, as well as the calibration of the model with subsequent statistical analysis of calibration outputs.

To create the model, it was first necessary to choose the correct spatial abstraction of the territory, determine the values of the input parameters, define the boundary conditions, and choose the appropriate time step. First, it was necessary to create a hydraulic model. This simulation was followed by heat transport model development. Using this model, it was possible to evaluate the impact of the Danube temperature and the air temperature in the aquifer. This model provided useful information on the changing groundwater temperature as well as the depth of its fixation at a constant temperature. These models were processed in the Groundwater Vistas 8 environment using the MODFLOW – USG program. With this modelling tool, it was possible to solve heat transport directly. The calculation was relatively fast and efficient, since many shortcomings had already been rectified by constant innovation and improvement of solution techniques.

The heat transport model was then important to verify, i.e., to determine the success of the calculation. The PEST calibration was used to verify the model. Calibration is a relatively complex and technically-demanding process. The aim of the calibration is to achieve the highest possible match between the calculated and measured parameters. To evaluate this compliance, the program has the option of displaying a graph that compares either the temperature or the groundwater level of the selected observation object. Calibration verification can also be performed through a set of statistical indicators. Certain limit values are determined for individual statistical indicators, for which the calibration is not sufficient, and it is necessary to repeat it. The pilot point method was also tested as part of the calibration process. Through these points, the hydraulic conductivity is characterized in more detail, which has a high impact on the resulting solutions.

Modelling is a complex method for which achieving a successful result involves a number of steps. However, it is possible to analyse a number of aspects from different angles, thereby making modelling a very useful and effective tool. The software equipment for the given issue is constantly being upgraded and improved, and its efficiency is continually enhanced. However, it is still a natural environment that will never be possible to simulate in its entirety.

In conclusion, it can be stated that by modelling heat transport in an aquifer, factors that lead to an increase in groundwater temperature can be identified either locally or regionally, and the time and depth development of temperature can be assessed. One of the disadvantages of modelling is a certain factor of subjectivity, especially when it is necessary to introduce simplifications for the calculation to be feasible. Modelling of natural processes is not possible for covering the whole complexity of the system, however, it provides a useful framework for quantification of temperature development or eventual prediction of development in the evaluated system.

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