

COMPARISON OF A BLACK-BOX MODEL TO A TRADITIONAL NUMERICAL MODEL FOR HYDRAULIC HEAD PREDICTION

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Received: 19/04/2016
Accepted: 28/06/2016
Available online: 19/10/2016

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ABSTRACT

Two different methodologies for hydraulic head simulation were compared in this study. The first methodology is a classic numerical groundwater flow simulation model, Princeton Transport Code (PTC), while the second one is a black-box approach that uses Artificial Neural Networks (ANNs). Both methodologies were implemented in the Bavaria region in Germany at thirty observation wells. When using PTC, meteorological and geological data are used in order to compute the simulated hydraulic head following the calibration of the appropriate model parameters. The ANNs use meteorological and hydrological data as input parameters. Different input parameters and ANN architectures were tested and the ANN with the best performance was compared with the PTC model simulation results. One ANN was trained for every observation well and the hydraulic head change was simulated on a daily time step. The performance of the two models was then compared based on the real field data from the study area. The cases in which one model outperforms the other were summarized, while the use of one instead of the other depends on the application and further use of the model.

Keywords: hydraulic head change simulation, groundwater modeling, Artificial Neural Network, Princeton Transport Code

1. Introduction

Various models have been used in the past to simulate the behavior of aquifers. Depending on their basis, they can be distinguished into three major categories, geomorphological, physically based and empirical. In brief, geomorphological models describe the dominant processes of a watershed and offer a close interpretation of the real world. The purpose of physically based models is to depict the underlying physics of the natural system. This type of models requires extensive knowledge of the physical characteristics of the system at study. The last category is empirical models, a main subcategory of which is black box models. These models rely on observation data with long time series of simple to acquire data, such as meteorological data (Pechlivanidis *et al.*, 2011).

Among the various model types, physically-based and black box models have been setup in different applications. In particular, the Princeton Transport Code (PTC) from the physically-based model group and the Artificial Neural Networks from the empirical model group have been favored. However, both models

have limitations depending on the modelling objectives. PTC is a classic numerical model that can only be used if geological information about the study area is available. While geological data are the cornerstone of this kind of models, if any other data are missing, assumptions can be made and data from nearby locations or neighbouring water bodies can be used with caution. In addition, the calibration process is time consuming and requires experience (both in terms of modelling and regional process understanding). However, after the successful calibration of the model, various scenarios can be studied concerning the aquifer parameters and the water management plans. On the contrary, ANNs do not require geological information, but they need long time series of data linked to the aquatic equilibrium. Without long time series of even a few parameters, it is impossible to train an ANN to identify patterns. ANNs can easily be implemented by non-experts, yet they can only be used for the study of parameters used during the training process. A basic assumption is that the effect of parameters for which data are not available is constant. This means that when data for one parameter are not available, it is not possible to study its effect on the aquifer or how it can change the simulation results if it differentiates.

The Princeton Transport Code (PTC) is a 3-D classical physically based numerical model which simulates the groundwater flow and transport of contaminants in porous media by combining the finite element and finite difference methods. It has been developed as a Plug-In Extension (PIE) for the ArgusOne GIS program (Babu *et al.*, 1987; Olivares, 2001). PTC uses partial differential equations to represent groundwater flow described by hydraulic head, groundwater velocity components and contaminant transport. A detailed description of the characteristics and functionality of PTC was presented in Babu *et al.*, (1987) and Pinder (2002). The main advantage in using numerical models is that, after being calibrated, a model can be used to simulate various scenarios and to study the impact of different management plans on the aquifer. On the downside, a wide range of data and parameter values must be available for the entire study area. The time and the expertise needed for the calibration of the boundary conditions is also a major drawback for this modelling technique.

PTC, together with Argus one, has been used in the past for groundwater simulation. In a study by Aivalioti and Karatzas (2006), it has been used in order to assess the impact of landfill leakage in the aquifer while in other studies it has been also used in order to determine the optimal water management scenario reducing saltwater intrusion (Papadopoulou *et al.*, 2007). Furthermore, PTC has been used in the past, together with optimization algorithms, in order to determine the optimal groundwater management scenario, which will reduce the contamination in a specific area (Karatzas *et al.*, 2007, Mergia and Kelly, 1994).

Artificial Neural Networks (ANNs) belong to the category of black-box models and have been proved to be an effective alternative to conventional groundwater modelling tool and a universal estimator (Tapoglou *et al.*, 2013; Trichakis *et al.*, 2011). An ANN is a system of interconnected basic components called neurons. The way these neurons (nodes) connect to each other, the number of layers and the number of nodes within these layers define the final architecture of the network. A detailed description of the functionality of ANNs was presented by ASCE Task Committee on Application of Artificial Neural Networks in Hydrology, (2000). ANNs can be used with the appropriate input parameters in order to simulate the aquatic equilibrium. The main advantage in using ANNs is that they do not require full geological characterization of the study area. On the other hand, they do require the use of long time series for all the data involved, which is the main disadvantage of this method (Haykin,1994).

ANNs have been extensively used in the past for environmental parameter simulation (Benvenuto and Marani, 2000), as well as for hydrological parameter determination (Lekkas *et al.*, 2004). In groundwater modelling, ANNs have been used in the past for temporal simulation of the hydraulic head (Trichakis *et al.*, 2009). They have also been used together with optimization algorithms in order to improve their results (Tapoglou *et al.*, 2013; Trichakis *et al.*, 2011) as well as for the spatiotemporal prediction of hydraulic head (Tapoglou *et al.*, 2014; Rizzo and Dougherty, 1994). An extensive review of applications of artificial neural networks in water resources is presented by Maier and Dandy (2000).

The scope of the present study is to setup two different types of models in area around Munich in Bavaria, Germany, and compare the results and the general functionality. The paper is organized as follows. A presentation of the models and the methodology of the experiment is presented in Section 2 followed by a description of the case study and data is presented in Section 3. Results are presented in Section 4, and finally Section 5 states the conclusions of this inter-comparison experiment.

2. Study area and data

The two methodologies were applied to an area around Munich in Bavaria, Germany. The study area covers approximately 2400 km² (Figure 1) and is dominated by Moraines and other Quaternary Pleistocene formations. The area has been studied on multiple occasions in the past, regarding both the quality and the quantity of the groundwater, due to its high significance. The hydraulic head can be characterized as medium to low, varying from 6.48 to 64.75 m d⁻¹ (Bender *et al.*, 2001; Heinrichs and Udkuft, 1999). The data available for this region spans a period from 1/11/2008 to 31/10/2012 (1456 days) and include daily time series of the hydraulic head in thirty (30) wells, the meteorological data from three weather stations (Augsburg, Munchen and Hohenpeibenberg), as well as the surface water elevation in two observation points (Munchen and Landshut Birket) across the Isar River (Figure 1). The meteorological data include series for average temperature, maximum and minimum daily temperature, daily snowfall, daily rainfall, wind speed and humidity.

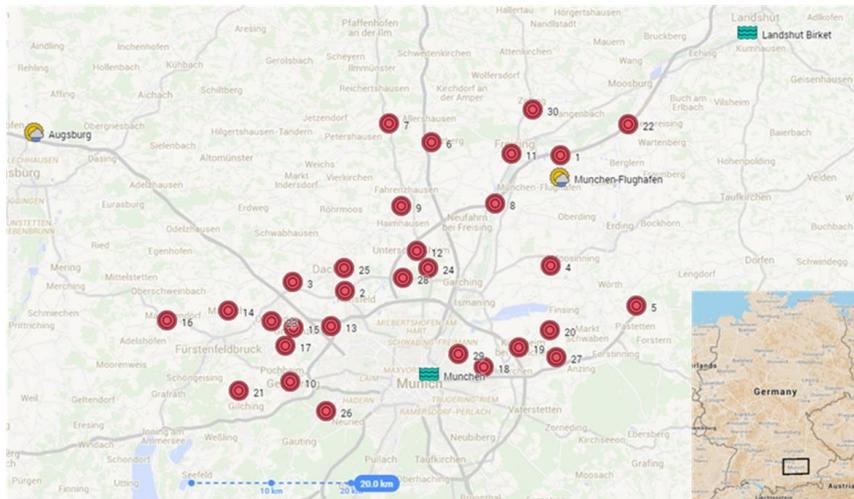


Figure 1. Study area (Google Maps, 2015)

The data concerning the hydraulic head in the wells, as well as the surface water levels, were made available through the Bavarian State Office for Environment (Bayerische Landesamt für Umwelt – BIfu), while the meteorological data were acquired from the German National Meteorological Service (Deutsche Wetterdienst-DWD).

3. Methodology

3.1. Groundwater simulation using PTC

The first model used for the hydraulic head simulation was the PTC. PTC uses as a basis the Darcy's law and the conservation of mass principles in order to simulate the groundwater flow in a study area (Babu *et al.*,

1987). More specifically a system of partial differential equations are solved by the code, in order to describe the hydraulic head (Eq. 1), and the velocity components (Eq. 2).

$$\frac{\theta}{\theta x} \left(K_{xx} \frac{\theta h}{\theta x} \right) + \frac{\theta}{\theta y} \left(K_{yy} \frac{\theta h}{\theta y} \right) + \frac{\theta}{\theta z} \left(K_{zz} \frac{\theta h}{\theta z} \right) - S \frac{\theta h}{\theta t} + Q = 0 \quad (\text{Eq. 1})$$

$$V_x = -K_{xx} \frac{\theta h}{\theta x}, \quad V_y = -K_{yy} \frac{\theta h}{\theta y}, \quad V_z = -K_{zz} \frac{\theta h}{\theta z} \quad (\text{Eq. 2})$$

where:

h : hydraulic head [L]

K_{xx}, K_{yy}, K_{zz} : hydraulic conductivity in x, y and z directions [$L T^{-1}$]

S : specific storage coefficient [L^{-1}]

Q : source / sink term [$L^3 T^{-1}$]

V_x, V_y, V_z : Darcy velocity x, y and z components [$L T^{-1}$]

θ : porosity (dimensionless)

Knowledge of parameters, such as hydraulic conductivity, rainfall-infiltration and porosity is necessary for the solution of Eq. 1 and 2. The elevation, the permeability and any known boundary conditions in the study area are also used by the model. The initial conditions concerning the hydraulic head can be determined through the available hydraulic head data.

In here, the simulation period is divided into three-month long stress periods. The results are presented as hydraulic head contour maps at the end of the stress period. Moreover the 4th stress period is used for model verification.

3.2. Groundwater simulation using ANNs

The second methodology relies on the use of ANNs for the temporal simulation of groundwater hydraulic head at multiple locations separately. One ANN was trained for every location and the available data. The ANNs were implemented in MATLAB, and in particular in the ANN toolbox and the Neural Network Fitting Tool (Demuth *et al.*, 2009). The Levenberg-Marquardt method was used for training as it can provide good training results with low computational cost (White, 1989).

The inputs for the ANNs were chosen by performing correlation analysis of the parameters under various time lags. All parameters linked to the aquatic equilibrium, such as rainfall, snowfall and surface water levels, can be used as inputs in the ANNs. Furthermore, the use of the hydraulic head value on the day before the one simulated as input parameter can improve the performance (Trichakis *et al.*, 2009). The architecture of the ANNs, i.e. the number of hidden layers and nodes within them, also plays a crucial role. In order to determine the number of nodes and hence the number of synaptic weights between them, a rule presented by Fine (1999) was used, according to which the number of synaptic weights capable of been adequately trained is the 1/3 of the total number of available datasets. Based on this rule, two architectures were examined in this study, the first with one hidden layer and the second with two hidden layers. The use of more than two hidden layers is not recommended as it adds considerable computational cost without furtherly improving the training result. In this way, the hydraulic head is simulated at multiple locations. In order to allow a comparison of the ANN results with those from the PTC model, the results were spatially interpolated for every time step.

3.3. Modelling parameters

The components of the water balance introduced to each model were related to the needs of each model separately. PTC needs geological meteorological and hydrological parameters, hence the conductivity of the

study area, porosity, rainfall, pumping activity were used. On the other hand, ANNs use data that can affect the hydraulic head and do not have constant values. For this reason rainfall, temperature relative humidity, hours of daily sunshine and surface water elevation data were used.

When PTC is used for the simulation of the hydraulic head, the characteristics of the study area are introduced to the model and the appropriate boundary conditions are manually calibrated through a trial and error process. The first parameter determined in the model is the hydraulic conductivity, derived by the hydrogeological maps of the region. Three main areas of hydraulic conductivity were identified: region 1 with hydraulic conductivity 64.75 m d^{-1} , region 2 with hydraulic conductivity 6.48 m d^{-1} , and region 3 with hydraulic conductivity 16.51 m d^{-1} (regions 1-3 are shown in Figure 2). The elevation as well as storativity and porosity in the study area were determined. The infiltration of the rainfall was set equal to 30% of the total precipitation at the Munich meteorological station and was calculated through the average daily rainfall for every stress period separately. Limited, not daily, pumping activity data were also available for the study area and were used as calibration parameters.

In ANNs, the choice of input parameters plays a crucial role in the performance of the simulation. All parameters with available data, which temporally vary and are linked to the water budget, can be used as input parameters. However, in order to reduce the complexity of the model, parameters that have low correlation with the hydraulic head itself must first be tested for their ability to improve the model. The use of snowfall as input parameter in the ANN development was questionable, since a large part of the time series has zero value, providing no pattern for the ANN to learn, while at the same time adding complexity to the model. Moreover, the correlation between snowfall and the hydraulic head change time series was low and the time lags considered very large. For this reason, two cases were studied, with and without the use of snowfall data. The following data were chosen as input for the simulation of the hydraulic head on day k : rainfall (four time series for four consecutive time lags), snowfall (three time series for consecutive time lags), surface water level (two time series for two consecutive time lags), temperature, relative humidity, hours of daily sunshine and hydraulic head on day $k-1$. This amounts to a total of thirteen (13) input parameters in the case where snowfall data is taken into consideration. Otherwise, the number of input parameters used is equal to ten. In both cases, the output parameter is the hydraulic head change per time step. The reason for using the hydraulic head change as output parameter instead of the hydraulic head itself is the high correlation between the hydraulic head on day k and on day, $k-1$, which can lead to high synaptic weights for this parameter, and thus diminishing the importance of the remaining parameters.

Two ANN architectures were tested in the case where snowfall data is taken into consideration: (a) an architecture with one hidden layer with 35 nodes, and, (b) an architecture with two hidden layers with 19 nodes in hidden layer 1 and 12 nodes in hidden layer 2. Similarly, two architectures were tested in the case without snowfall data: (a) an architecture with one hidden layer with 44 nodes, and, (b) an architecture with two hidden layers with 20 nodes in hidden layer 1 and 13 nodes in hidden layer 2.

4. Results

4.1. PTC results

As a first step, all the necessary data are imported to Argus one - PTC PIE, including the hydraulic conductivity, initial conditions, meteorological data and infiltration and available pumping rates. The calibration of the model was performed by trial and error, using type 1 and type 2 boundary conditions. Wells with known hydraulic head, in close proximity to the domain outline, were used as type 1 boundary conditions. All other wells with known hydraulic head values within the study area were used in the calibration process and for the verification of the model. The initial hydraulic head at locations where data were available was set equal to the value on the first day of the simulation. Linear interpolation was used to determine the initial hydraulic

head at locations throughout the study area where data were not available. In the perimeter of the study area other type 1 and 2 boundary conditions were introduced, representing the inflow and outflow of the water. Moreover, taking into consideration the limited pumping activity data available and their location, type 2 boundary conditions were also introduced inside the study area. Unknown or uncertain, due to data availability, boundary conditions were calibrated in order to improve the simulation and validation results. For the validation of the model, the simulation at the end of the 1st simulation year (4th stress period) are calculated and depicted in Figure 2.

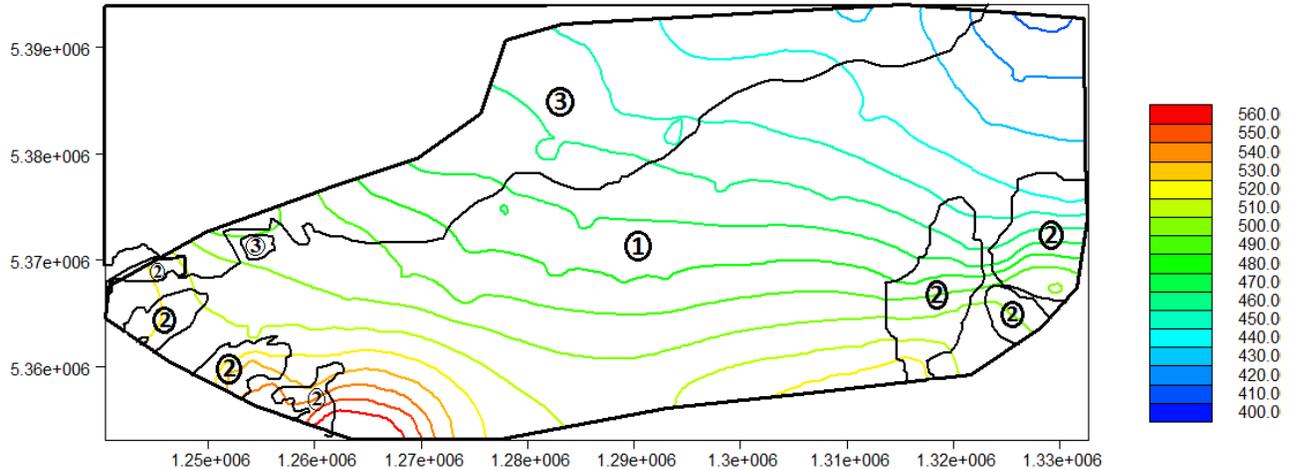


Figure 2. Hydraulic head contours at the end of the 4th stress period evaluated by using PTC

Various error indicators were calculated for the evaluation of the derived results. These error indicators used the hydraulic head data recorder in the field in the thirty wells with available data and the simulated values at the exact same locations. The Nash-Sutcliffe efficiency (Nash and Sutcliffe, 1970), which has proved very effective for hydrological data, was calculated equal to 0.98, while the mean absolute relative error (MARE) equal to $0.62 \cdot 10^{-2}$. These values indicate the successful modelling and simulation by using PTC. The average deviation between observed and simulated values at locations where data were available, calculated equal to 1.5 m, can be considered low, considering the complexity of the study area and the lack of pumping activity data.

4.2. ANN results

The parameters defined through the training process are the synaptic weights connecting the nodes of each ANN layer to the ones on the next layer.

Table 1. Characteristic MSE values for simulations which include snowfall

	One hidden layer			Two hidden layers		
	Training Error (m ²)	Testing Error (m ²)	Evaluation Error (m ²)	Training Error (m ²)	Testing Error (m ²)	Evaluation Error (m ²)
Mean	$9.79 \cdot 10^{-4}$	$1.19 \cdot 10^{-3}$	$1.40 \cdot 10^{-3}$	$9.27 \cdot 10^{-4}$	$1.42 \cdot 10^{-3}$	$1.19 \cdot 10^{-3}$
Maximum	$2.67 \cdot 10^{-3}$	$3.12 \cdot 10^{-3}$	$3.22 \cdot 10^{-3}$	$2.00 \cdot 10^{-3}$	$2.95 \cdot 10^{-3}$	$3.41 \cdot 10^{-3}$
Minimum	$3.25 \cdot 10^{-4}$	$4.43 \cdot 10^{-4}$	$3.55 \cdot 10^{-4}$	$3.73 \cdot 10^{-4}$	$3.67 \cdot 10^{-4}$	$3.44 \cdot 10^{-4}$
Overall Mean	$1.19 \cdot 10^{-3}$			$1.18 \cdot 10^{-3}$		

After the training process is completed three types of errors can be calculated training error, which corresponds to the error at the training dataset, testing error which corresponds to the error in the testing

dataset and validation error. Simulation results for four separate cases are summarized in terms of mean squared error (MSE) in Table 1 and 2. The results presented in Table 1 are for the ANN architectures that include snowfall as input parameter, whereas the results presented Table 2 are for the case where snowfall is ignored.

As expected, the use of snowfall as an input parameter did not improve the ANN performance. Between the ANN architectures that did not use snowfall data, the architecture with one hidden layer resulted in slightly better performance and will be used henceforth.

Table 2. Characteristic MSE values for simulations which do not include snowfall

	One hidden layer			Two hidden layers		
	Training Error (m ²)	Testing Error (m ²)	Evaluation Error (m ²)	Training Error (m ²)	Testing Error (m ²)	Evaluation Error (m ²)
Mean	$1.03 \cdot 10^{-3}$	$8.73 \cdot 10^{-4}$	$9.11 \cdot 10^{-4}$	$9.48 \cdot 10^{-4}$	$6.47 \cdot 10^{-4}$	$1.24 \cdot 10^{-3}$
Maximum	$1.94 \cdot 10^{-3}$	$2.06 \cdot 10^{-3}$	$2.79 \cdot 10^{-3}$	$1.88 \cdot 10^{-3}$	$1.70 \cdot 10^{-3}$	$2.11 \cdot 10^{-3}$
Minimum	$4.01 \cdot 10^{-4}$	$3.97 \cdot 10^{-4}$	$3.90 \cdot 10^{-4}$	$3.46 \cdot 10^{-4}$	$3.93 \cdot 10^{-4}$	$4.70 \cdot 10^{-4}$
Overall Mean	$9.38 \cdot 10^{-4}$			$9.44 \cdot 10^{-4}$		

For the presentation of the derived simulation results, the 30 wells/data points were organized into three categories (groups) according to performance in terms of average training, testing and evaluation error. Wells that belong to the same category have similar performance. Results are presented for one representative well from each group, the one that has the average performance in its group. Wells with poor performance results were included in group 1, while those with best performance results were included in group 3. The results for the representative wells from each group are summarized in Table 3.

Table 3. Characteristic values for the representative wells

	Representative wells		
	Group 1 (well no. 23)	Group 2 (well no. 25)	Group 3 (well no. 6)
Absolute value of difference between real and simulated HHC			
Average (m)	$1.23 \cdot 10^{-2}$	$9.86 \cdot 10^{-3}$	$6.69 \cdot 10^{-3}$
Minimum (m)	$9.71 \cdot 10^{-6}$	$1.09 \cdot 10^{-5}$	$3.45 \cdot 10^{-6}$
Maximum (m)	$3.15 \cdot 10^{-1}$	$1.43 \cdot 10^{-1}$	$1.72 \cdot 10^{-1}$
ANN MSE error			
Training (m²)	$1.15 \cdot 10^{-3}$	$8.10 \cdot 10^{-4}$	$4.60 \cdot 10^{-4}$
Testing (m²)	$8.48 \cdot 10^{-4}$	$5.67 \cdot 10^{-4}$	$3.97 \cdot 10^{-4}$
Evaluation (m²)	$1.03 \cdot 10^{-3}$	$6.54 \cdot 10^{-4}$	$4.44 \cdot 10^{-4}$

Simulation results for the hydraulic head change per time step for the three representative wells are presented in Figure 3.

Simulation results for the hydraulic head change were derived for all 30 wells with data available. The hydraulic head per time step for each well in the field was calculated from the hydraulic head change results and the initial hydraulic head value. The hydraulic head contours were generated by using the Argus One environment and the linear interpolation method. The results for the hydraulic head at the end of the 1st simulation year (corresponding to the 4th stress period in PTC) are depicted in Figure 4.

4.3. Model intercomparison - Discussion

The choice of model depends on the scope of the simulation. ANNs yield better performance in the case where accurate point simulations are required. In the case of spatial simulations, the accuracy of the model depends on the interpolation method applied. PTC and other classic numerical models can result in better overall performance for spatial simulation, but lack accuracy in the case of point simulation. Their overall

performance depends on the calibration process, which can be a time-consuming and sometimes a difficult process.

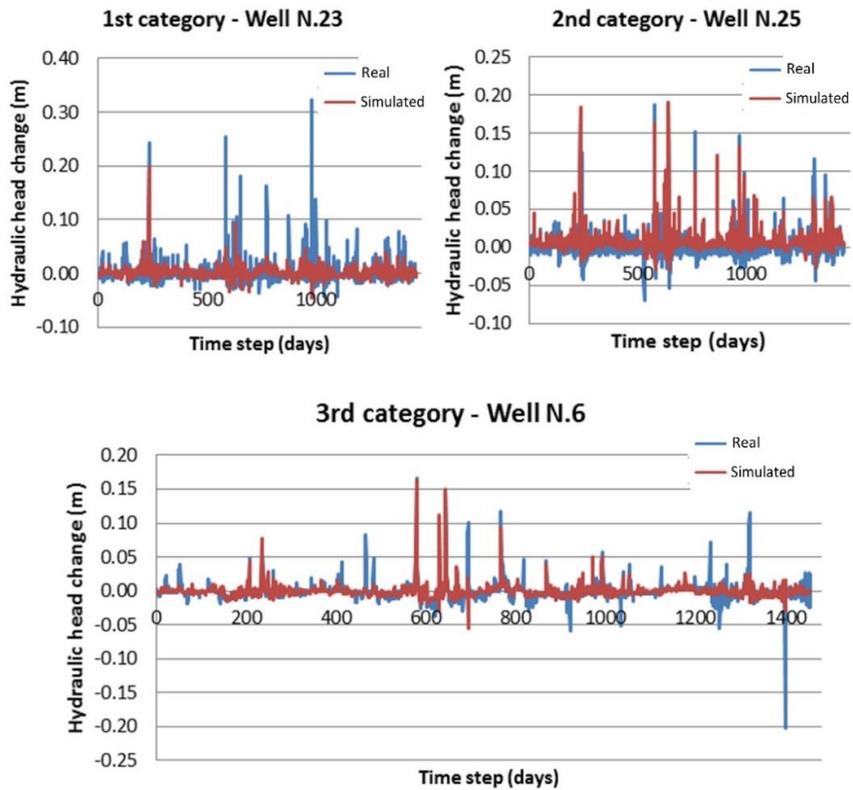


Figure 3. Hydraulic head change per time step for wells No. 23, 25 and 6 using ANNs

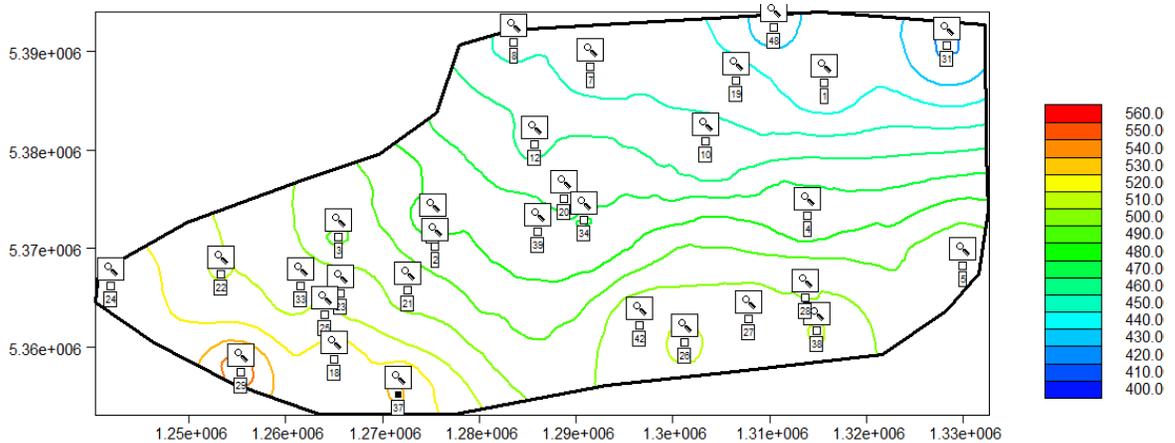


Figure 4. Hydraulic head contours at the end of the 1st simulation year evaluated by using ANNs

Another factor that determines the choice of model is the data availability. ANNs require long time series of easily available data. Meteorological, surface water and pumping data can all be used, as long as they are available. There is no requirement for specific essential data, on the contrary, all available data related to the water budget can be used. PTC, on the other hand, requires a smaller amount of data than ANNs, which,

however, are more expensive to collect, if not available. Geological data such as hydraulic conductivity and porosity and information about boundary conditions are necessary for the construction of the PTC model.

In every case, the decision upon the use of each model depends on the purpose of the study and their further use. After a successful calibration process, numerical models, such as PTC, can be used to study various water management and climate change scenarios. In many cases these kind of models are used to examine the effect of alteration of pumping activity or climate change in the aquifer. When using black box models, like ANNs, it is only possible to examine the effect of alteration of parameters which are used as inputs to the model. In order to study the effect of any other parameter on the simulation results, a new training of the ANNs is necessary, incorporating data for this parameter.

In order to achieve the best possible simulation results within the objective of a study, all the advantages and limitations of both models should be considered in order to use the most appropriate type of model.

5. Conclusions

In this paper, two different methodologies, one based on the numerical model PTC and one using artificial neural networks, were applied for the hydraulic head simulation in a study area around Munich in Germany. Results for the hydraulic head at the end of the 1st simulation year were presented for the comparison of the two models. Both models are capable of providing good performance results for the simulation of the hydraulic head. In the case of ANNs, the average MSE at locations with data available was equal to $9.38 \cdot 10^{-4} \text{ m}^2$, while in the case of, PTC the average deviation between observed and simulated values was equal to 1.5 m. This difference can be attributed to the fact that in PTC the hydraulic head is simulated, while in ANNs the hydraulic head change per daily time step is studied.

While both modelling methods have both advantages and disadvantages, the final selection of the most appropriate is based on the purpose of the study at hand and the data availability. If the management of the groundwater in the study area is the goal of the study, numerical models are more appropriate, while if precision at a specific location is of essence, ANNs can yield better results. Moreover, if the geology of the study area is not specified in detail or the spatial variability is high ANNs may be more appropriate, while if long time series of data are not available, numerical models are more accurate.

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