Numerical modeling of the interaction river-aquifer and solute transport simulations

Uncertainty in river boundary conditions during extreme flood events

Scientific work to obtain the grade of
M.Sc. Environmental Engineering

Department of Civil, Geo and Environmental Engineering
Technical University of Munich

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Declaration of Authorship

I hereby declare that this Master’s Thesis titled “Numerical modeling of the interaction river-aquifer and solute transport simulations: Uncertainty in river boundary conditions during extreme flood events” has been composed by me and is based on my own work, unless stated otherwise. This Master’s Thesis was not previously published or presented to another examination board.

Date: ___________________________  Signature: ___________________________

Pablo Merchán-Rivera
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Abstract

NUMERICAL MODELING OF THE INTERACTION RIVER-AQUIFER AND SOLUTE TRANSPORT SIMULATIONS: UNCERTAINTY IN RIVER BOUNDARY CONDITIONS DURING EXTREME FLOOD EVENTS

by Pablo Merchán-Rivera

Flood events can greatly influence the dynamic of groundwater flow and the interactions between aquifers and streams. In groundwater modeling, extreme events represent a transient state in the boundary conditions which may affect the groundwater flow and the transport of solutes of the modeled system. In addition, the estimation of hydrological extreme events is complex and affected by major uncertainties. These uncertainties may affect the results of numerical models. A three-dimensional numerical model of the groundwater flow of the valley of Tacherting was developed using MODFLOW-2005 to describe the groundwater flow under flood conditions, and advective and dispersive transport of solutes was simulated using MT3DMS. Lastly, the associated uncertainty with the river stage and the riverbed conductance was evaluated simulating different scenarios. Strong interrelationships were observed between the aquifer and the streams during the simulation period. Changes in both velocity and direction of the flow were detected at different phases of the flood event. The uncertainty in the river conditions is larger during the peak of the flood event and it influences the overall results of the numerical simulations. River boundary conditions control the aquifer responses in the proximities of the streams and the relative importance of uncertainties relies on spatial and temporal considerations.

Key words: groundwater modeling, solute transport simulation, uncertainty, parameter estimation, sensitivity, flood events, river boundary conditions, stream-aquifer interaction.
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1. Introduction

Groundwater represents about 98% of the freshwater in the planet (Margat & van der Gun, 2013), and it is an essential component of the hydrological cycle. As part of the continuous cycle of water, groundwater is not independent of surface water bodies, and the interactions between groundwater and surface water occur in nearly all landscapes, from small streams, lakes, and wetlands to major river valleys and seacoasts (Winter, 1999). The interaction mechanisms must be understood for managing effectively water resources; however, they are complex and dynamic due to geomorphologic, hydrogeologic, and climate controls (Sophocleous, 2002). These interactions are of paramount importance for understanding the fate and transport of solutes. In fact, the physical, chemical and biological mechanisms which intervene in the migration, degradation and remediation of contaminants may be highly affected by the interaction of groundwater and surface water.

The exchange between the stream and aquifers can highly vary at different temporal and spatial scales (Schmadel, Ward, Lowry, & Malzone, 2016). Moreover, extreme events, such as floods or droughts, can greatly influence the dynamic of groundwater flow fields and the interrelationships between groundwater and streams. The high stages of flow that overtop the banks of river and channels during flood events (Das & Saikia, 2009; Deodhar, 2008) are normally characterized by the peak of flow rate, flood elevation, flood volume or flood duration (Raudkivi, 2013). For instance, major floods may dramatically change the spatial extent of hyporheic zone and the direction of subsurface flow paths, altering both the hydrologic residence time of water in the hyporheic zone and the rate of hyporheic exchange flow (Wondzell & Swanson, 1999); precipitation events and seasonal climatic patterns alter hydraulic head and may induce variations in flow direction, changing effluent and influent conditions (Sophocleous, 2002); rivers lose water to bank infiltration during floods, reducing flood level and recharging aquifers (Brunke & Gonser, 1997; Sophocleous, 2002), and also they induce both pressure and solute movement into aquifers at different ranges (Welch, Cook, Harrington, & Robinson, 2013).

For understanding these hydrogeological systems, it is essential to apply a quantitative analysis of groundwater flow through groundwater numerical models. Since any hydrogeological models face uncertainty, which reduces its applicability and confidence, the quantification of the
uncertainty is a crucial step. The results due to uncertainty in models of flow and transport can often improve through inadequacy studies (Beven & Westerberg, 2011; Ye, Neuman, & Meyer, 2004). New methods and tools for calibrating models and analyzing uncertainty are transforming the science of groundwater (Anderson, Woessner, & Hunt, 2015) through the development of theoretical and computational frameworks incorporating uncertainties in the parameters and models (Bolster et al., 2009; Tartakovsky, 2007).

In groundwater modeling, extreme events represent a transient state in the boundary conditions affecting the water and solute exchange between surface water and groundwater (Brunner, Simmons, Cook, & Therrien, 2010; Sophocleous, 2002). Since extreme events are affected by major uncertainties and their estimations are also complex (Apel, Thieken, Merz, & Blöschl, 2004; Beven & Binley, 1992), the uncertainty quantification must be considered when models of the interaction groundwater-surface water are performed. The quantification of uncertainties is also essential for solute and contaminant fate and transport, because it is often required to identify the magnitude, size and duration of them in the system (Mattis, Butler, Dawson, Estep, & Vesselinov, 2015).

The relative roles of dynamic hydrologic forcing and geomorphology that control the timescales and magnitudes of exchange stream-aquifer are unknown (Schmadel et al., 2016). Additionally, despite the high influences of flood events in the groundwater regime, the interactions between streams and the aquifer during these extreme periods have not been deeply studied. Similarly, only few studies consider the evaluation of the uncertainty of river boundary conditions during flood events. Consequently, this study aims to estimate the impact of river boundary conditions on the interaction between groundwater and surface water during flood events. A substantial aspect of this work is the evaluation of the uncertainties related to the river which can affect the results of numerical modeling and consequently the simulation of solute transport. Additionally, the research also introduces one study case in the scientific understanding of groundwater flow and the transport of solutes in the porous medium, under the consideration of the effects of flood events and the interaction between surface water and the groundwater regime.

Therefore, this study develops a three-dimensional numerical model of the groundwater flow of the valley of Tacherting to describe the groundwater flow under flood conditions, and evaluate the associated uncertainty due to river boundary conditions not only for the groundwater flow simulation, but also for the simulation of solute transport. The simulation was performed using MODFLOW-2005 (Harbaugh, 2005) as code for solving the finite-difference model, and Processing Modflow version 8.0 (Chiang, 2011; Simcore Software, 2012) as the graphical user interface. The USGS particle-tracking code MODPATH (Pollock, 1994) is used to generate the advective pathlines of water particles and their associated travel time based on MODFLOW.
simulations. Finally, the study includes the simulation of advective and dispersive transport of a hypothetical solute using MT3DMS (C. Zheng & Wang, 1999).

The valley of Tacherting (Bavaria, Germany), where the Alz river and the Alz channel flow, is largely composed by gravel deposits derived from melted water pathways of central Alpine glaciers (Doppler et al., 2011), which allow a very dynamic groundwater flow (Keilholz, Kumar, & Disse, 2015). In May and June 2013, heavy rainfalls caused the rising of both stream stages and groundwater levels which affected the municipality (Gemeinde Tacherting, 2017b), especially due to the seepage of groundwater into buildings (Disse, Keilholz, & Kumar, 2015). Keilholz et al. (2015) developed three-dimensional groundwater models for Tacherting (large scale) and the village of Wajon (small scale) for the investigation of basic stage flood. The existing research and the dataset from Keilholz et al. (2015) are used as the basis of this study for evaluating the dynamics of the hydrological processes of the flood event in Tacherting. No additional technical surveys were performed in this study, and the update of the model is based only on previous studies. The level of detail is determined and adjusted by the modeling purpose, the practical limits during the development of the numerical model and the available field data. The limitations and simplifications assumed in this study are those commonly related to groundwater modeling by underlying simplifying approximations, and by nonuniqueness and uncertainty.
2. Theoretical Framework

2.1. Basics of hydrology and hydrogeology

2.1.1. Groundwater and the hydrologic cycle

The continuous cycle of water through the land and atmosphere by a series of transformations is known as the hydrologic cycle (cf. Figure 2:1), and it consists of inflows, outflows, and storage. (Babar, 2005). The driving force of this natural circulation is derived from the radiant energy from the Sun, and the pathways for water transformation are evaporation, condensation, and precipitation (Shaw, Beven, Chappell, & Lamb, 2010). Figure 2:1 describes the continuous movement of the water in the hydrologic cycle.

![Figure 2:1. The hydrologic cycle and its components (from Bear, 2007)](image)

The last paragraph conveys to a basic concept in hydrology: the water budget. It refers to the amount of water entering, stored within, and leaving a hydrologic system (Babar, 2005; S. Wang et al., 2014). The various components which are part of the water budget can be included in a
mathematical way in the *water balance equation*, which is based on the principle of conservation of mass (cf. Chapter 2.3.2). The understanding of regional water budget is actually a powerful tool for water resource management, flood control, pollution control, groundwater recharge estimation, among others (S. Wang et al., 2014). Since the volume of soil may be chosen arbitrary, ranging from a small sample to an entire catchment, the decision will depend on the purpose of the investigation (Zhang, Walker, & Fleming, 2002).

On one hand, groundwater is an ordinary component of the hydrological cycle, and it is not independent of the other components of the cycle. Moreover, an estimated of eight to ten million cubic kilometers of fresh groundwater represents about 98 to 99% of all liquid freshwater on the planet (Margat & van der Gun, 2013). On the other hand, groundwater is the mechanical cause of geologic, geomorphologic, and physiographic phenomena, and it also serves as the vehicle for both natural and mineral matter, and liquid substances (Tóth, 1970). The natural storages of underground water are the pores, fissures, and fractures of the strata of the Earth’s crust (Shiklomanov & Rodda, 2003).

Groundwater derives mostly from both percolation of precipitation and surface water of streams and lakes that supply water to *aquifers* (Kresic, 2006) when it sweeps downward into the subsurface through the porous of the soil (Cech, 2010). Aquifers are hydraulically continuous bodies of relatively permeable porous or fissured rocks, which contain groundwater, whereas *aquitards* or *aquicludes* are groundwater filled bodies of poorly permeable formation. The comparatively high permeability of aquifers allows the flow of groundwater. Aquitards may hold large volumes of groundwater and exchange them with the aquifers, through large surfaces of contact (Margat & van der Gun, 2013).

Aquifers can be classified according to the absence or presence of water table as *confined* or *unconfined*, respectively. A confined aquifer is bounded by impervious formations from above and below. When the elevations of the piezometric surface\(^1\) in a confined aquifer are above the ground surface is called *artesian aquifer*. On the other hand, unconfined aquifers are those where the water table or piezometric surface serve as its the upper boundary. These aquifers may be recharged from the surface if there is no impervious layers in between (Bear, 1988, 2007). The Figure 2:2 briefly illustrates the aquifer types.

---

1 Piezometric surface is the imaginary surface defined by the water levels in observation wells tapping a certain aquifer. It is also known as isopiestic surface (Bear, 1988)
There is an important differentiation between two zones in the subsurface: the *saturated zone* and the *unsaturated zone*. The area below the water table is denoted as the saturated zone and the soil at elevations above the water table is denoted as unsaturated or vadose zone (Pinder & Celia, 2006). This is crucial for the explanation of flow and mass transport in the future. The water movement through saturated porous materials can mainly be described by Darcy’s Law (K. A. Smith & Mullins, 2001) (cf. Chapter 2.3.1), whereas the understanding of unsaturated zone flow is more complicated because of the presence of air and water in the pore space (Fetter, 1999) and the simultaneous flow of these two immiscible fluids (Bear, 1988).

Three types of groundwater flow systems can be distinguished according to Tóth (1963): *local*, *intermediate*, and *regional*. Local systems are characterized by flows to nearby discharge areas (e.g., streams). Differently, regional flows systems discharge in major rivers, large lakes or oceans, after traveling greater distances. Intermediate flow systems are mainly characterized by one or more topographic highs and lows although its recharge and discharge areas do not occupy the highest and lowest elevated places. Sophocleous (2002) gives an accurate review of the principal geomorphologic, hydrogeologic, and climatic controls on groundwater flow systems. He states that groundwater flow systems are controlled by the difference in topography and the consequent difference in potential; the configuration of the water table and the hydraulic conductivity; and, climate, being the precipitation the main source of groundwater recharge.
2.1.2. Surface water and groundwater interactions

The geographical distribution of groundwater is related to the geological structure of the Earth crust and climatic factors such as precipitation, condensation, evaporation, and particularly infiltration. There is a strong link between groundwater and surface runoff, starting from the fact that both of them depend on the same hydrological factors (Shiklomanov & Rodda, 2003). Groundwater and surface water are not isolated components of the hydrologic system. They actually interact in a variety of physiographic and climatic landscapes. These interactions between groundwater and surface water are complex, and in order to understand their relation to climate, landform, geology, and biotic factors, an ample knowledge of hydrogeological conditions is necessary (Sophocleous, 2002).

Tóth (1970) considers that the hydrogeological conditions are composed of physical and chemical parameters enclosed in two groups: hydrogeologic environment and groundwater regime. The components of the hydrogeologic environment include topography, geology, and climate; whereas the second, the groundwater regime, comprises the amount of water, the geometric distribution of the groundwater movement, the volume or velocity of the flow, chemical composition, temperature, and regime variance. Particularly, three characteristics govern the interaction of streams, lakes, and wetlands with groundwater: the position of the water bodies with respect to groundwater flow systems; the geologic characteristics of their beds; and, their climatic settings (Sophocleous, 2002; Winter, 1999). The hydrologic interactions between surface and subsurface waters occur by infiltration into or exfiltration from the saturated zones and by subsurface lateral flow through the unsaturated soil (Sophocleous, 2002). The infiltration rate depends upon soil texture, the degree of compaction, and ambient moisture content (Hudak, 2000).

Various mechanisms describe the flow interactions between rivers and aquifers. In general terms, the river may contribute water to the aquifer or serve as its drain. Indeed, much of the baseflow² is derived from groundwater whose hydraulic head elevations are higher than the head in the stream. In this case, we refer to effluent streams. On the contrary, when the water level of the stream is higher than the hydraulic head of the aquifer is called influent stream (Bear, 2007). To assume any of these interactions, it is clearly important to firstly recognize if the free surface on a groundwater intercepts the water level in the channel. If this is the case, they are hydraulically connected. The stream-aquifer system is hydraulically disconnected when there are unsaturated media between the channel and the water table (Stephens, 1995). These interrelationships are explained in Figure 2:3.

² Baseflow is the portion of a watercourse flow received by the stream that is attributed to groundwater seeping (Poehls & Smith, 2011).
An important component for analyzing the interaction of aquifers and rivers is the *hyporheic zone*. It is defined as the area of active mixing between groundwater and surface water found in the unconfined near-stream aquifers (Wondzell & Swanson, 1999). This region has been recognized due to its importance for the ecosystem functions (e.g., Brunke & Gonser, 1997), and, lately, many professionals have been overlooked, because the state of the science has not been transferred to the practice (Lawrence et al., 2013), particularly during hydrologic extreme events (Doble, Crosbie, Smerdon, Peeters, & Cook, 2012).

### 2.1.3. Flood events

Extreme events, such as floods or droughts, are rare and unusual events defined as extreme due to their great magnitude or the length of duration (Jones, 2014). By definition, a flood is a high stage of flow that overtops the banks of rivers and channels (Das & Saikia, 2009; Deodhar, 2008) and may be characterized by the peak of flow rate, flood elevation, flood volume and flood duration (Raudkivi, 2013). But also, floods can occur when the water level in lakes, ponds, reservoirs, estuaries, sea surges or aquifers exceed some critical value causing the inundation of the adjacent land (Şen, 2017).

Damages due to floods can be distinguished in terms of infrastructure, private property, and public safety (F. Zheng, Sebastian, & Bedient, 2014). Since floods are considered the most dangerous weather-related events (Şen, 2017; Z. Y. Wang, Lee, & Melching, 2014; F. Zheng et al., 2014), flood forecasting has become into a well-developed activity (Rodda & Robinson, 2015). An important role has been played by the statistics of extremes, which nowadays includes trends in hydrologic extremes due to climate change (Katz, Parlange, & Naveau, 2002).
The influence of the interaction of geomorphic and hydrologic controls onto stream-aquifer exchange may highly vary at different temporal and spatial scales (Schmadel et al., 2016). Extreme events can modify the prescribed perceptions of the standard hydrological conditions. For instance, major floods may dramatically change the spatial extent of hyporheic zone and the direction of subsurface flow paths, altering both the hydrologic residence time of water in the hyporheic zone and the rate of hyporheic exchange flow (Wondzell & Swanson, 1999); the movement of water and sediments in rivers and streams modifies the landscape, especially during flood periods, streams and river act as erosive agents (Babar, 2005); and, rivers lose water to bank infiltration during floods, reducing flood level and recharging aquifers (Brunke & Gonser, 1997; Sophocleous, 2002).

2.1.4. Groundwater contamination and contaminant migration

During the twentieth century, groundwater has received unprecedented stress from the exploitation activities and pollution in both developed and developing countries (Margat & van der Gun, 2013). There are many potential sources of groundwater contamination. Fetter (1999) lists some of the most frequent sources, as well as identified contaminants. Among the sources are landfills, injection wells, hazardous-waste sites, land application, saltwater intrusion, agricultural activity storage, septic tanks, and pits from oil and gas wells. Since the potential sources are diverse, there is a wide variety of material that includes: hydrocarbons, metals, and cations, nonmetals and anions, microorganisms, radionuclides.

Gravity, pressure, and friction determine the groundwater movement. Even if the main difference between groundwater and surface water flow is that the groundwater flow is slower (Rail, 2000), groundwater contamination is a complex problem because of its long-term nature and the difficulty to be discovered (Fetter, 1999). Therefore, the location and extension of pollution is a key element for the assessment of the conditions of water. In general, there are two mechanisms that control the fate of a contaminant: transformation processes and transport mechanisms. The first involves the transformation of compounds due to chemical reaction, and the second one includes mechanisms as the advective transport and dispersive transport (Schnoor, 1996).

The contamination concerns about groundwater have motivated the use of groundwater flow and contamination transport models, as well as the development of computer simulation models (Rail, 2000). The understanding of the basic principles of the interaction and interchange of groundwater and surface water is needed for an effective management of water resources (Winter, 1999) and it requires a quantitative framework that allows conceptualizing the hydrogeologic processes (Anderson et al., 2015).
2.2. Principles and properties of groundwater flow

2.2.1. Aquifer properties

The capability of aquifers for storing, transmitting, and yielding groundwater is governed by several properties, such as porosity, effective porosity, intrinsic permeability, hydraulic conductivity, transmissivity, specific yield, and storage coefficient (Hudak, 2000). These are briefly reviewed in this section, including the mathematical statements for their calculation.

**Porosity and effective porosity**

The void fraction or empty spaces in the subsurface is known as *porosity*. It is represented by \( n \) in the context of void ratio \( e \), as follows:

\[
e = \frac{V_v}{V_s},
\]

\[
n = \frac{V_v}{V} = \frac{V_v}{V_s} = \frac{e}{1 + e},
\]

where \( V_v \) is the volume of the void space; \( V_s \) is the volume of solid grains; and, \( V \) is the denominator that considers changes as the soil compacts or consolidates (Pinder & Celia, 2006).

The *effective porosity*, \( n_e \), is the interconnected pore space available for fluid flow (Wiedemeier, 1999). It cannot exceed the total porosity (cf. Table 2:1):

\[
n_e < n.
\]

**Table 2:1. Representative porosity values for well-sorted unconsolidated formation (Modified from Morris & Johnson, 1967)**

<table>
<thead>
<tr>
<th>Material</th>
<th>Diameter [mm]</th>
<th>Total porosity [%]</th>
<th>Effective porosity [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gravel</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarse</td>
<td>64,0-16,0</td>
<td>28</td>
<td>23</td>
</tr>
<tr>
<td>Medium</td>
<td>16,0-8,0</td>
<td>32</td>
<td>24</td>
</tr>
<tr>
<td>Fine</td>
<td>8,0-2,0</td>
<td>34</td>
<td>25</td>
</tr>
<tr>
<td>Sand</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coarse</td>
<td>2,0-0,5</td>
<td>39</td>
<td>27</td>
</tr>
<tr>
<td>Medium</td>
<td>0,5-0,25</td>
<td>39</td>
<td>28</td>
</tr>
<tr>
<td>Fine</td>
<td>0,25-0,162</td>
<td>43</td>
<td>23</td>
</tr>
<tr>
<td>Silt</td>
<td>0,062-0,004</td>
<td>46</td>
<td>8</td>
</tr>
<tr>
<td>Clay</td>
<td>&lt;0,004</td>
<td>42</td>
<td>3</td>
</tr>
</tbody>
</table>
Permeability and hydraulic conductivity

Some media are characterized by high porosity but low permeability due to the small sizes of the pores or their poor connection. Therefore, the porosity is considered an insufficient condition for transmitting fluids (Hudak, 2000). However, the intrinsic permeability, $\kappa$, is the property that relates to the ability of the medium to transmit fluids (Lal & Shukla, 2004). For example, zones of high permeability in the subsurface function as drains (Freeze & Witherspoon, 1967).

The coefficient of proportionality, $K$, known as hydraulic conductivity, is defined as the measure of the ability of the porous media to transmit water. It can have different values in the three principal directions $K_x$, $K_y$, and $K_z$ if the medium is anisotropic, or the equal value all directions, $K_x = K_y = K_z = K$, if the medium is considered isotropic (Fetter, 1999). Figure 2.4 shows typical values of hydraulic conductivity and permeability according to soil type.

The difference between intrinsic permeability and hydraulic conductivity is that the permeability is property solely of the porous medium, whereas the hydraulic conductivity is a property of both the fluid and the porous medium (Lal & Shukla, 2004). They can be related through the following expression (Nutting, 1930):

$$K = \frac{\kappa \rho g}{\mu}$$

where $\kappa$ is the intrinsic permeability [L$^2$]; $K$ is the hydraulic conductivity [LT$^{-1}$]; $\mu$ is dynamic viscosity of the fluid [ML$^{-1}$T$^{-1}$]; $\rho$ is the water or fluid density [ML$^{-3}$]; and, $g$ is the acceleration of gravity.

![Figure 2.4. Typical values of hydraulic conductivity and permeability (Bear, 1988)](image)

---

3 A medium is anisotropic when the ease of flow differs depending the direction (Pinder & Celia, 2006).

4 A medium is called isotropic when the flow is equally easy in all directions (Pinder & Celia, 2006).
Hydraulic head and hydraulic gradient

The hydraulic head, \( h \), also known as the piezometric head, is the sum of the elevation above the datum, \( Z \), and the pressure head term, \( h_p \). Neglecting the groundwater velocity because in most cases is very low, the hydraulic head can be defined as (Kresic, 2006):

\[
h = Z + h_p = Z + \frac{p}{\rho g}
\]

in which the pressure head \( h_p \) is represented by the pressure of the fluid, \( p \), over a constant density \( \rho \) times the acceleration of gravity, \( g \).

The hydraulic gradient, \( I \) [-], is the difference of the hydraulic head between two points, \( h_1 \) and \( h_2 \) [L], divided by the distance, \( l \) [L], between these two points (Hudak, 2000):

\[
I = \frac{\Delta h}{l} = \frac{h_1 - h_2}{l}
\]

There is an inherent heterogeneity at pore size dimensions that can occur at different scales (e.g., particle, aggregate, field and regional). This heterogeneity implies a variation in the soil properties. Therefore, the objective measurements of hydraulic conductivity is to enable the quantitative prediction of fluid flow under the given conditions (K. A. Smith & Mullins, 2001).

Transmissivity

The transmissivity, \( T \) [L^2/T], is the rate of flow per unit width through the entire thickness of an aquifer per unit of the hydraulic gradient (Bear, 2007). Therefore, it is equal to the integral of the hydraulic conductivity times the aquifer thickness, \( B \), or roughly (Charbeneau, Bedient, & Loehr, 1992):

\[
T = K \times B
\]

Aquifer storativity

As Johnson (1967) explains, not all the water contained in the saturated zone can be removed by drainage or by pumping wells. There is a part retained by molecular surface tension forces in the voids of the soil. Two terms describe the water-yielding capacity and the water-retaining capacity. The term specific yield, \( S_y \), is used to define the volume of water drained from a soil column of unit cross-sectional area per unit decline in the elevation of the water table, while the volume of the remaining water is denoted as \( S_r \) and is called specific retention, (Pinder & Celia,
2006). The terms are often expressed in percentage. Table 2.2 shows estimated values of the specific yield of various soil materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>Maximum [%]</th>
<th>Minimum [%]</th>
<th>Average [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>5</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Silt</td>
<td>19</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>Sandy clay</td>
<td>12</td>
<td>3</td>
<td>7</td>
</tr>
<tr>
<td>Fine sand</td>
<td>28</td>
<td>10</td>
<td>21</td>
</tr>
<tr>
<td>Medium sand</td>
<td>32</td>
<td>15</td>
<td>26</td>
</tr>
<tr>
<td>Coarse sand</td>
<td>35</td>
<td>20</td>
<td>27</td>
</tr>
<tr>
<td>Gravelly sand</td>
<td>35</td>
<td>20</td>
<td>25</td>
</tr>
<tr>
<td>Fine gravel</td>
<td>35</td>
<td>21</td>
<td>25</td>
</tr>
<tr>
<td>Medium gravel</td>
<td>26</td>
<td>13</td>
<td>23</td>
</tr>
<tr>
<td>Coarse gravel</td>
<td>26</td>
<td>12</td>
<td>22</td>
</tr>
</tbody>
</table>

As is shown in (Bear, 2007), it is possible to link the specific yield and the total porosity, as follow:

\[ n = S_y + S_r. \]  \[8\]

In three-dimensional transient flow problems, it is also necessary to consider the volume of water released from or taken into storage per unit volume of porous medium, which is the specific storage, \( S_s \, [\text{L}^1] \) (Johnson, 1981). It is given as (Kresic, 2006):

\[ S_s = \rho g(\alpha + n_e \beta), \]  \[9\]

where \( \rho \) is the mass density of water \([\text{ML}^{-3}]\), \( g \) is the gravitational acceleration \([\text{LT}^{-2}]\), \( \alpha \) is aquifer (or aquitard) compressibility \([\text{T}^2\text{LM}^{-1}]\), \( n_e \) is effective porosity \([\text{c}]\), and \( \beta \) is the compressibility of water \([\text{T}^2\text{LM}^{-1}]\) equivalent to \(4.4 \times 10^{-10} \text{m s}^2/\text{kg}\).

<table>
<thead>
<tr>
<th>Material</th>
<th>Specific storage ([\text{m}^{-1}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plastic clay</td>
<td>(2.0 \times 10^3 - 2.6 \times 10^3)</td>
</tr>
<tr>
<td>Stiff clay</td>
<td>(2.6 \times 10^3 - 1.3 \times 10^4)</td>
</tr>
<tr>
<td>Medium-hard clay</td>
<td>(1.3 \times 10^3 - 9.2 \times 10^4)</td>
</tr>
<tr>
<td>Loose sand</td>
<td>(1.0 \times 10^4 - 4.9 \times 10^4)</td>
</tr>
<tr>
<td>Dense sand</td>
<td>(2.0 \times 10^4 - 1.3 \times 10^4)</td>
</tr>
<tr>
<td>Dense sandy gravel</td>
<td>(1.0 \times 10^5 - 4.9 \times 10^5)</td>
</tr>
<tr>
<td>Rock, fissured, jointed</td>
<td>(6.9 \times 10^5 - 3.3 \times 10^6)</td>
</tr>
<tr>
<td>Rock, sound</td>
<td>(&lt; 3.3 \times 10^5)</td>
</tr>
</tbody>
</table>
The *storativity* (also known as *storage coefficient*) is a parameter of the storage function of an aquifer (Watson & Burnett, 1995). It relates the changes in the quantity of water stored in an aquifer with the changes in the piezometric surface (in confined aquifers) or the water table (in unconfined aquifers) (Bear, 1988). Equations 10 and 11 define the storativity, $S [-]$, for confined and unconfined aquifers, respectively. Both transmissivity and storativity can only be determined in the field through pumping tests (Watson & Burnett, 1995).

\[
S = S_s B , \tag{10}
\]

\[
S = S_y + S_s B . \tag{11}
\]

### 2.3. Governing equations of groundwater flow

#### 2.3.1. Darcy’s Law

Through an experiment, based on a saturated sand-filled column, Henry Darcy (1856) specified the flow rate of water entering the top and draining from the bottom of the column. He found that the one-dimensional flow of water through the column of sand was proportional to the cross-sectional area and the head loss along the column and inversely proportional to the flow length. This is called *Darcy’s Law*, and can be expressed as:

\[
Q = -KA \frac{dh}{dl} , \tag{12}
\]

in which $Q$ is the volumetric discharge; $K$ is the proportionality constant known as hydraulic conductivity; $A$ is the cross-sectional area; and, $dh/dl$ is the gradient of the hydraulic head. Dividing by the cross-sectional area, it is possible to express the equation in terms of *specific discharge* or *Darcy’s flux*, $q$, as follow:

\[
q = -K \frac{dh}{dl} . \tag{13}
\]

The simple mechanism described by equation 13 can be used to represent both baseflow and river recharge and are illustrated in Figure 2:5.
Figure 2.5. Various mechanisms describing flow between river and aquifer (Sophocleous, 2002): a) the mechanisms for flow from the aquifer to the river (baseflow) and from the river to the aquifer (river recharge) are the same; b) the rate of flow from the river to the aquifer is slower than the rate of flow from the aquifer to the river; c) no flow can occur from the river to the aquifer; d) nonlinear relationship; and, e) combination of linear and nonlinear relationship.

As is explained by Fetter (1999), in order to describe mathematically a 3D groundwater flow, the scalar, vector and tensor properties of hydraulic head and hydraulic conductivity must be defined. As was mentioned previously in this Chapter, if the medium is anisotropic, the hydraulic conductivity can have different values depending upon the actual direction $x$, $y$, and $z$. Therefore, it can be described as a tensor, $K$, of nine components:

$$K = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix}.$$  \[14\]

Considering a symmetric tensor, if the coordinate system is oriented along the principal axis, we assume a diagonal structure and obtain the simplest form of the tensor $K$:

$$K = \begin{bmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{bmatrix}.$$  \[15\]
Although Darcy’s Law was specified for one-dimensional flow, the head is also a function of all three dimensions \( h = h(x, y, z) \). Therefore, the gradient of the head, \( \nabla h \), is a vector, with magnitude and direction. The specific discharge can be represented as a vector, \( \mathbf{q} \), then:

\[
\mathbf{q} = -\mathbf{K} \cdot \nabla h ,
\]

Therefore, the three components of the specific discharge vector, \( \mathbf{q} \), are the following:

\[
q_x = -K_{xx} \frac{\partial h}{\partial x} - K_{xy} \frac{\partial h}{\partial y} - K_{xz} \frac{\partial h}{\partial z} ,
\]

\[
q_y = -K_{yx} \frac{\partial h}{\partial x} - K_{yy} \frac{\partial h}{\partial y} - K_{yz} \frac{\partial h}{\partial z} ,
\]

\[
q_z = -K_{zx} \frac{\partial h}{\partial x} - K_{zy} \frac{\partial h}{\partial y} - K_{zz} \frac{\partial h}{\partial z} .
\]

2.3.2. Continuity equation for groundwater hydraulics

The law of mass conservation states that the mass of a system must remain constant over the time. Zhang, Walker, & Fleming (2002) explain this in a very simple form saying that the water balance states that any change in water content of a given volume of soil, during a specified period, must be equal to the amount of water added to the volume of soil minus the amount of water that is withdrawn of it. The mathematical statement of the law of conservation of mass is called continuity equation (Charbeneau et al., 1992), and there are four key elements to describe it: control volume; inputs and outputs; transport characteristics within the control volume and across the boundaries; and, reaction kinetics (Schnoor, 1996).

As is presented by Fetter (1999), the derivation of the flow equation can be explained through a control volume, generally known as representative elementary volume (REV). Therefore, we refer no net change in the mass of fluid in a small REV of a porous medium (cf. Figure 2:6). In Figure 2:6, \( dy \, dz \) is the area of the two faces normal to the \( x \) axis; \( dx \, dz \) is the area of the two faces normal to \( y \); and, \( dx \, dy \) is the area of the two faces normal to \( z \).

\[^{5}\] In mechanics of continuous media, the representative elementary volume is the characteristic volume in which is possible to take average values of microscopic quantities to define macroscopic physical variables (e.g., pressure, temperature, velocity and density) avoiding relative high fluctuations due to inhomogeneities in the medium (Guyon, 2001).
Thus, the total net mass accumulation within the control volume is:

\[
\text{Total net mass accumulation} = - \left[ \frac{\partial}{\partial x} (\rho q_x) + \frac{\partial}{\partial y} (\rho q_y) + \frac{\partial}{\partial z} (\rho q_z) \right] dx \, dy \, dz . \tag{20}
\]

Considering that the change in mass of water with respect to time, \( \partial M / \partial t \), is:

\[
\frac{\partial M}{\partial t} = \frac{\partial}{\partial t} (\rho m \, dx \, dy \, dz) , \tag{21}
\]

and, assuming that the fluid may change with respect to time and that the coordinate system is aligned with the principal axes of anisotropy, we can substitute Darcy’s Law for the components of the specific discharge, we obtain:

\[
\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) = \frac{1}{\rho} \frac{\partial}{\partial t} (\rho m) . \tag{22}
\]

Finally, expressing the right side of the equation as the specific storage times the change in the head with respect to time, we obtain the partial differential equation for transient flow in an anisotropic medium parallel to the major axes of hydraulic conductivity:

\[
\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) = S_s \frac{\partial h}{\partial t} . \tag{23}
\]
We can include the volumetric flux per unit volume representing sources and/or sinks of water, represented as \( W \) [T\(^{-1}\)]:

\[
\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) + W = S_s \frac{\partial h}{\partial t}.
\]

[24]

2.3.3. Solute transport in porous media

The transport of solutes in porous media is also known as mass transport and, similarly to the groundwater flow, can be described by means of partial differential equations. The transport of conservative solutes\(^6\) can be basically described by advection, dispersion, and diffusion. Advection is the bulk (large-scale) movement described mathematically by the fluid’s velocity (Hemond & Fechner, 2015) produced when groundwater moves and carries with it dissolved constituents (Charbeneau, 2006). Dispersive transport is the spreading of a solute along and across the main flow direction due to aquifer heterogeneities at pore scale and macroscale (Delleur, 1999). Finally, molecular diffusion corresponds to an increase in entropy when dissolved substances move from the region of high concentration to regions of low concentration, and it is defined as the mixing of dissolved chemicals caused by the random walk of molecules within the fluid. (Schnoor, 1996).

Mechanical dispersion and molecular diffusion are intimately related and cannot be separated in groundwater flows. They can be combined to define the hydrodynamic dispersion coefficient, \( D \). The dispersion coefficient may be evaluated according to its direction with respect to the direction of the flow for accounting the effects of spatial differences in velocities, as follow:

\[
D_L = \alpha_L \bar{v}_i + D^*,
\]

[25]

\[
D_T = \alpha_T \bar{v}_i + D^*,
\]

[26]

where \( D_L \) is the longitudinal hydrodynamic dispersion [L\(^2\)T\(^{-1}\)]; \( D_T \) is the transverse hydrodynamic dispersion [L\(^2\)T\(^{-1}\)]; \( \alpha_L \) and \( \alpha_T \) are the dynamic dispersivity terms [L]; \( \bar{v}_i \) the average linear velocity in the \( i \); and, \( D^* \) is the effective diffusion coefficient (Bear, 1972).

---

\(^6\) Conservative solutes are those which do not interact with the porous media or decay biologically or radioactively (Fetter, 1999).
The advective transport and the dispersive transport (cf. Figure 2.7) of a solute in the $i$ direction can be summed to find the total mass of solute per unit cross-sectional area per unit time, $F$, as follow:

$$F_i = \underbrace{v_i n_i C}_{\text{advective transport}} \underbrace{- n_i D_i (\frac{\partial C}{\partial t})}_{\text{dispersive transport}}.$$

[27]

Bear (1972) describes the development of the partial differential equation governing advective-diffusive transport. Considering the conservation of mass and the rate of mass change in a representative elementary volume, the three-dimensional equation of mass transport can be written as:

$$\frac{\partial C}{\partial t} = \left[ D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \right] - \left[ v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \right],$$

[28]

where $\partial C / \partial t$ is the change in concentration with respect to time [ML$^{-1}$T$^{-1}$]; $D_x$, $D_y$, and $D_z$ are the dispersion coefficient considering the direction components $x$, $y$ and $z$; and, $v_x$, $v_y$, and $v_z$ are the average linear velocities with the direction components $x$, $y$ and $z$.

By adding a new term, $r_m$, the advection-dispersion-reaction-equation can be expressed. This term is the net contribution of physical, chemical, and biological reaction rates [ML$^{-3}$T$^{-1}$]. Additionally, the term $R$ was also added to represent the retardation factor and to describe the interaction between the solute and the solid phase of the porous medium. Therefore, for one-dimensional transport, we obtain:

$$R \frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_x \frac{\partial^2 C}{\partial x^2} \pm \Sigma r_m.$$

[29]
2.4. Groundwater modeling

The quantitative framework, which is necessary for understanding the hydrological process, can be provided with a hydrological model. The groundwater modeling process follows the scientific method, where a question is asked, a hypothesis is constructed and tested, and, finally the hypothesis is accepted or rejected (Anderson et al., 2015). This process is schematized in Figure 2:8.

![Figure 2:8. Modeling process (from Bear & Cheng, 2010)](image)

By definition, a model is a simplified version of a real system, which approximately simulates the excitation-responses relationships of interest (Bear & Cheng, 2010). A groundwater model provides quantitative evidence for conceptualizing hydrogeologic processes or for synthesizing field information (Anderson et al., 2015). This is essential in hydrogeology, because in groundwater regimes it is practically impossible to observe separately all the phenomena connected. Therefore, the importance of the model relies on its capacity to separate the different features of the system and draw particular attention on the most relevant properties (Tóth, 1963).

Many classifications have been constructed to organize the mathematical modeling process. Mathematical models are classified as *black-box models* if they use empirical or statistical equations derived from the available data for calculating the unknown variables, or, as *process-
based models if they use processes and principles of physics to represent the groundwater flow. These process-based models can also be segmented in stochastic or probabilistic, depending if they use (stochastic) or not (deterministic) any of their parameters have a probabilistic distribution. But also, mathematical models can be also subdivided according to the method of solution. Analytical solutions provide general solutions that can be applied to various domains and parameters, whereas numerical methods will transform the mathematical model into a numerical one (Bear & Cheng, 2010).

2.5. Numerical models

Most of the time, analytical solutions of the partial differential equation for transient flow are not possible. It is convenient to apply methods of numerical analysis to obtain approximated solutions. Therefore, partial differential equations are solved transforming them into finite-dimensional subspaces by discretization. The most common methods for groundwater modeling are the Finite-Difference Method and the Finite-Element Method, which differ in concept, but they may yield similar results for the groundwater governing equation (Anderson et al., 2015).

The Finite-Element Method solves differential equations through the subdivided series of elements of simple shapes (e.g., triangular, quadrilateral, and rectangular) to represent the solution domain (Huyakorn, 2012). In contrast to the Finite-Difference Method, which solves the dependent variable at the nodes, the Finite-Element Method defines the dependent variable as a continuous solution within elements (Anderson et al., 2015).

2.5.1. Finite-Difference Method

In general, the Finite-Difference Method is simply and efficient for providing adequate numerical solutions of partial differential equations, and the given solutions are as accurate as the data warrant and as accurate as is required from the technical point of view. It gives approximate solutions because that the derivative at a point are approximated by difference quotients over a small interval (G. D. Smith, 1985). This means that the fundamental principle of the method consists in the replacement of derivatives of a function $u$ at a discrete point $(x = a)$ by the difference of the values of the function $u$ at a point $a - \Delta x/2$ and $a + \Delta x/2$ dividing by the spacing of those points, which reads:

$$
\frac{du}{dx} = \lim_{\Delta x \to 0} \frac{\Delta u}{\Delta x} \approx \frac{u_a - u_{a+\Delta x}}{\Delta x}.
$$

[30]
The Finite-Difference Method needs to replace the region over which the independent variables in the partial differential equations are defined by *grid* or *mesh*, where the dependent variable is approximated (Causon & Mingham, 2010). In this method, *nodes* are located in 3D space and indexed to assign relative locations (Anderson et al., 2015).

The Finite-Difference approach is explained more in detail in accordance with the scope of this research, relating its computation to the application in MODFLOW (Harbaugh, 2005) for solving the governing flow equation. Therefore, the detailed description of the numerical model in the next sections follows that presented by Harbaugh (2005), unless expressly stated otherwise. Also, notice that a different indexing convention and mathematical notation can be found in different sources.

2.5.2. MODFLOW and the groundwater flow process

The numerical code MODFLOW uses a finite difference approach to model groundwater flow. The first version was published in 1984 and it was released solely as only as a groundwater-flow simulation code (McDonald & Harbaugh, 1984). MODFLOW is the USGS’s modular hydrologic model and it has become the industrial international standard for groundwater modeling because of its flexible modular structure, complete coverage of hydrogeological processes and public domain free availability (Zhou & Li, 2011). Nowadays, numerous programs have been developed to solve additional related equations. For instance, the 2005 version, MODFLOW-2005, includes the simulation of saturated-unsaturated flow process, groundwater simulation-optimization process, irrigation process, density dependent flow process, parameter optimization process and solute transport process (Barlow & Harbaugh, 2006).

As was introduce beforehand, the solution of equation 25 requires to replace the continuous system by a finite set of discrete points in space and time. The system is expressed with an array of blocks called *cells* located in terms of rows, columns and layers. The hydraulic heads are calculated within each cell, where a point called *node* is placed. To assign a relative location, the nodes are located in 3D space by the indices \((i, j, \text{ and } k)\), which represent row, column, and layer (respectively).

Since the continuity law states that all flows into and out of the cell must be equal to the rate of change in storage within the cell, and, assuming that the density of the groundwater is constant, the groundwater flow equation in finite-difference form can be written as:

\[
\Sigma Q_i = SS \frac{\Delta h}{\Delta t} \Delta V, \tag{31}
\]
where $Q_i$ is a flow rate into the cell [L$^3$T$^{-1}$]; SS is the equivalent notation in for specific storage in the finite-difference formulation, which means the volume of water that can be injected per unit volume of aquifer material per unit change in head [L$^{-1}$]; $\Delta V$ is the volume of the cell [L$^3$]; and $\Delta h$ is the change in head over a time interval of length $\Delta t$. So, the volume of water entering in the storage over a time interval $\Delta t$ given $\Delta h$ is the term on the right-hand. Outflow is represented as negative inflow and losses as negative gain. Flow from cell $i,j-1,k$, into a cell $i,j,k$ is given by Darcy’s law (equation 13):

$$q_{ij-1jk} = K R_{ij-1jk} \Delta c_i \Delta v_k \frac{(h_{ij-1,k} - h_{ij,k})}{\Delta r_{j-1k}} ,$$

[32]

where $h_{ij,k}$ is the head at node $i,j,k$ and $h_{ij-1,k}$ is the head at node $i,j-1,k$ [L]; $q_{ij-1jk}$ is the volumetric flow rate through the face between cells $i,j,k$ and $i,j-1,k$ [L$^3$T$^{-1}$]; $K R_{ij-1jk}$ is the hydraulic conductivity along the row between nodes $i,j,k$ and $i,j-1,k$ [L$^3$T$^{-1}$]; $\Delta c_i \Delta v_k$ is the area of the cell faces normal to the row direction; and, $\Delta r_{j-1k}$ is the distance between nodes $i,j,k$ and $i,j-1,k$ [L]. Similar expressions are used for the remaining faces in the different directions, where the notations are analogous to equation 33, and they vary according to directions, cells, faces and nodes.

MODFLOW allows to represent different features through the addition of terms. This means the addition of terms for flows into the cell from features or processes external to the aquifer (e.g., rivers, drains, areal recharge, evapotranspiration, or wells). The flows may be entirely independent of the head in the receiving cell or dependent on the head in the receiving cell but independent of all other heads in the aquifer. These terms are $P_{ij,k}$ and $Q_{ij,k}$ represents the flow from the $n^{th}$ external source into cell $i,j,k$ [L$^3$T$^{-1}$]. If we consider equation 33 and, also, that the flows from the six adjacent cells, change in storage, and the external flow rate, we obtain:

$$q_{ij-1jk} + q_{ij+1jk} + q_{i-1jk} + q_{i+1jk} + q_{ij,k-1} + q_{ij,k+1} + P_{ij,k} h_{ij,k} + Q_{ij,k}$$

$$= SS_{ij,k} \left( \Delta r_j \Delta c_i \Delta v_k \right) \frac{\Delta h_{ij,k}}{\Delta t} ,$$

[33]

where $\Delta h_{ij,k}/\Delta t$ [LT$^{-1}$] is a finite-difference approximation for the derivative of head with respect to time; $SS_{ij,k}$ represents the specific storage of cell $i,j,k$ [L$^{-1}$]; and $\Delta r_j \Delta c_i \Delta v_k$ is the volume of cell $i,j,k$ [L$^3$].
The finite-difference approximation for the time derivative of head, \( \Delta h_{ijk}/\Delta t \), has to be expressed in terms of specific heads and times. Therefore, the approximation to the time derivative of head at time \( t^m \) is obtained as:

\[
\frac{\Delta h_{ijk}}{\Delta t} \approx \frac{h_{ijk}^m - h_{ijk}^{m-1}}{t^m - t^{m-1}}. \tag{34}
\]

MODFLOW applies an iterative process to get the solution to the system of finite-difference equations for each time step. An arbitrarily value for the head at each node at the end of the time step is given for the calculation of heads. New outcome values are produced in sequence until the system of equations is satisfied. The most common indirect method used to define when to stop iterating is the closure criterion or convergence criterion. It consists on the specification, by the user, of a certain quantity and the changes in computed heads from one iteration level to the next must be less than this.

There are two main types of packages in MODFLOW: internal and stress packages. The internal package simulates the flow between adjacent cells. On the other hand, the stress packages simulate individual types of stress (e.g., rivers, wells and recharge). The solution methods are called solver packages. Table 2:4 shows a list of packages of MODFLOW and indicates the package category of each one. Some of these are important for this research and are revised below for a better understanding.

*Table 2:4. List of Packages for simulating ground-water flow (Harbaugh, 2005)*

<table>
<thead>
<tr>
<th>Package Name</th>
<th>Abbreviation</th>
<th>Package Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basic</td>
<td>BAS</td>
<td>Program Control</td>
</tr>
<tr>
<td>Block-Centered Flow</td>
<td>BCF</td>
<td>Hydrologic/Internal</td>
</tr>
<tr>
<td>Layer-Property Flow</td>
<td>LPF</td>
<td>Hydrologic/Internal</td>
</tr>
<tr>
<td>Horizontal Flow Barrier</td>
<td>HFB</td>
<td>Hydrologic/Internal</td>
</tr>
<tr>
<td>Well</td>
<td>WEL</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>Recharge</td>
<td>RCH</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>River</td>
<td>RIV</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>General-Head Boundary</td>
<td>GHB</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>Drain</td>
<td>DRN</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>Evapotranspiration</td>
<td>EVT</td>
<td>Hydrologic/Stress</td>
</tr>
<tr>
<td>Strongly Implicit Procedure</td>
<td>SIP</td>
<td>Solver</td>
</tr>
<tr>
<td>Preconditioned Conjugate Gradient</td>
<td>PCG</td>
<td>Solver</td>
</tr>
<tr>
<td>Direct Solution</td>
<td>DE4</td>
<td>Solver</td>
</tr>
</tbody>
</table>
The Layer-Property Flow (LPF) and Block-Centered Flow (BCF) packages are internal flow packages that provide alternate approaches to simulate the internal flow terms. The difference between them is the input data that each of them require, but the conceptualization is identical. LPF package allows to define layers as confined and convertible. In convertible layers, the transmissivity varies and are computed during each solver iteration. Also, there is the possibility to convert a cell to no flow when head goes below bottom elevation

**Time- Variant Specified-Head:**

The Time-Variant Specified-Head (CHD) was originally developed by Leake & Prudic (1991). The aim of this option is to designate different constant head cells within or between stress periods, which makes changing the head at constant-head cells throughout a simulation possible. It is considered as part of the Basic Package (BAS) due to its function for designating constant-head cells.

**Recharge package**

The stress packages formulate the coefficients for describing a particular external or boundary flow. One of this is the Recharge Package (RCH), which simulates distributed recharge to the groundwater system. This means that the package allows to represent recharge in the top layer as result of percolation into the aquifer at different time periods, applying it in one single cell. The calculation of the recharge applied is defined as follow:

\[
QR_{ij} = I_{ij}DELR_jDELC_i, \tag{35}
\]

where \(QR_{ij}\) is the recharge flow rate applied to the model at horizontal cell location \([LT^{-1}]\); and \(I_{ij}\) is the recharge flux \([LT^{-1}]\); and, \(DELR_jDELC_i\) represent the value of the horizontal cell area \([L^2]\).

**River package**

The River Package (RIV) simulates effects of flow between surface water streams and the groundwater system. The package calculates the flow between the river and the aquifer, \(Q_{riv}\) \([LT^{-1}]\), applying equation 36 when \(h_{ijk} \leq RBOT_n\) or equation 37 when \(h_{ijk} > RBOT_n\):

\[
Q_{riv} = CRIV_n(HRIV_n - RBOT_n), \tag{36}
\]

\[
Q_{riv} = CRIV_n(HRIV_n - h_{ijk}), \tag{37}
\]
in which \( R_{BOTn} \) is the elevation of the bottom of the riverbed; \( HRIV \) is the water level or stage in the river \([L]\); \( h_{ij,k} \) is the head at the node in the cell underlaying the river reach \([L]\); and, \( CRIV \) is the hydraulic conductance of the river-aquifer interconnection \([L^2T^{-1}]\), computed as:

\[
CRIV_n = \frac{K_n L_n W_n}{M_n},
\]

where \( L \) is the length of the river as it crosses the node \([L]\); \( W_n \) is the river width \([L]\); \( M_n \) is the thickness of the riverbed layer \([L]\); and, \( K_n \) is the hydraulic conductivity of the riverbed material \([LT^{-1}]\).

2.5.3. MODPATH and particle tracking

The simulation of particle traces and their corresponding travel times, known as particle tracking, is a common technique in groundwater hydraulics, which also allows to understand the advective transport of solutes. Particle tracking helps to identify recharge and discharge areas; contributing areas to rivers, lakes, and springs and capture zones of pumping wells; and assess the effects of partially penetrating wells and streams (Anderson et al., 2015). The tool has been applied for instance, to visualize cells which act as weak sinks or sources (e.g., Abrams, Haitjema, & Kauffman, 2012); for analysis of river-aquifer interaction (e.g., Abdel-Fattah, Langford, & Schulze-Makuch, 2008; Shamsuddin, Suratman, Zakaria, Aris, & Sulaiman, 2014); and, to determine the seasonal variation in residence times in aquifers (e.g., des Tombe et al., 2016).

A widely-used code for particle tracking is MODPATH (Pollock, 1994). This code is particle tracking post-processing package that uses the cell-by-cell flows and potentiometric heads generated by the numerical groundwater flow model MODFLOW (Harbaugh, 2005; McDonald & Harbaugh, 1984). Pollock (1994) describes in detail the functionality of the code. MODPATH uses a semi-analytical particle tracking scheme to express the flow paths of the particles within each finite-difference grid cell. The user can designate the location of fictitious particles and the period of time for performing the transport through the flow field of MODFLOW.

MODPATH computes its track until the particles reaches a boundary, an internal source or sink, or a specific termination criterion. For this purpose, MODPATH firstly determines the face across which the particle leaves a cell using the velocity components at the different faces by solving a simple linear interpolation. Then, it evaluates the required time for the particle to reach the possible exit faces. Therefore, the coordinates of the particle \((x_p, y_p, z_p)\) at any future time \((t_2)\) can be computed by:
\[ x_p(t_2) = x_1 + \left( \frac{1}{A_x} \right) \left[ v_{x_p}(t_1)e^{(A_x \Delta t)} - v_{x_1} \right], \]  
\[ y_p(t_2) = y_1 + \left( \frac{1}{A_y} \right) \left[ v_{y_p}(t_1)e^{(A_y \Delta t)} - v_{y_1} \right], \]  
\[ z_p(t_2) = z_1 + \left( \frac{1}{A_z} \right) \left[ v_{z_p}(t_1)e^{(A_z \Delta t)} - v_{z_1} \right], \]

in which \( \Delta t \), equal to \( t_2 - t_1 \), is the time required for the particle to reach a possible exit face; \( A_x, A_y \) and \( A_z \) are constants that correspond to the components of the velocity gradient within the cell; \( v_{x_1}, v_{y_1} \) and \( v_{z_1} \) are the average linear velocity components across each face; \( v_{x_p}, v_{y_p} \) and \( v_{z_p} \) are the coordinate components of velocity for the particle; and, \( x_p, y_p \) and \( z_p \) are the components of the location of the particle denoted by the coordinate \( x, y \) and \( z \). The sequence of calculations is applied cell by cell until the particle reaches a termination criterion and the approach is generalized by MODPATH to describe the particle movement in three-dimensional domains.

2.5.4. MT3DMS and solute transport modeling

The importance and mathematical basis of the solute modeling for fate and transport of contaminants was described previously (cf. Chapter 2.3.3). The set of options of numerical codes that can simulate solute transport is diverse. As well as the groundwater flow, the basis of simulation codes is the application of numerical methods to solve the governing equations, in this case the advection-dispersion-reaction-equation which describes the fate and transport of contaminants. MT3DMS is a modular multispecies transport model code to simulate advection, dispersion, diffusion, and chemical reactions of contaminants in groundwater flow systems (C. Zheng & Wang, 1999).

One of the features of MT3DMS is that the code interfaces directly with MODFLOW (Harbaugh, 2005; McDonald & Harbaugh, 1984). MT3DMS can be used with any block-centered finite-difference flow model. The code assumes that changes in the concentration field will not significantly affect the flow in the system. Among the solution techniques in the code, MT3DMS includes the fully implicit finite difference method (FDM), the particle-tracking based method of characteristics (MOC) and its variants (modified MOC and hybrid MOC), and a third-order total variation diminishing (TVD) scheme that conserves mass while limiting numerical dispersion and artificial oscillation (C. Zheng, Hill, Cao, & Ma, 2012; C. Zheng & Wang, 1999).

For transport modeling using MT3DMS the basic calibrated parameters needed are the hydraulic conductivity, storage properties, dispersion values, and porosity. It is possible to simulate dual-
domains (mobile and immobile domains) adding rate coefficients. Furthermore, the code can simulate reactive transport if sorption or chemical reaction rate constants are included (C. Zheng et al., 2012).

2.6. Uncertainty Analysis

Relatively simple flow governing equations conceptualize the natural hydrological processes in groundwater model (cf. Chapter 2.2). But, groundwater systems are complex, and the results of groundwater simulations often deviate from true values due to uncertainty of numerical simulations. Models are uncertain owing to our inability to fully represent the hydrogeological system (Anderson et al., 2015). By definition, uncertainty is referred to any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system (Walker et al., 2003).

Groundwater is influenced from very diverse hydrological and meteorological conditions, geological structure, topography features, vegetation, human activities, and more, which may signify a source of uncertainty (Wu & Zeng, 2013). Furthermore, in practical situations, aquifer characteristics such as conductivity, porosity, depth, and geometry are never exactly known, and measurement can be expensive and be affected by observation error (Van Lent & Kitanidis, 1989). Among these conditions, as was reviewed in the chapter 2.1, it is important to include the effect of extreme events (such as floods, droughts and storm surge), which are also affected by major uncertainties and their estimations are complex too (Apel et al., 2004; Beven & Binley, 1992). Anderson et al. (2015) exemplify some aleatory and epistemic uncertainties in hydrologic modeling, which are summarized in Table 2:5.

Since uncertainty has been recognized to limit the applicability of groundwater modeling results, theory and application of statistics and probabilistic concepts in groundwater systems have emerged to assess uncertainty (Anderson et al., 2015). A large number of publications about the applied statistics in hydrogeology can be found (e.g., Gelhar, 1993; Kitanidis, 1997; Rubin, 2003) as well as a large number of approaches for uncertainty classification have been proposed (e.g., Yen, 1986; Merz & Thieken, 2009). Uncertainties are normally associated with model conceptualization, particular spatial parameterization scheme, numerical issues for spatial and temporal discretization, and, last but not least, limitations in expert knowledge and a paucity of measurement data (Sepúlveda & Doherty, 2015).
As Freeze et al. (1990) state, this innate uncertainty of numerical models should be quantified and incorporated into the framework for hydrogeological decision analysis. For this purpose, uncertainty in groundwater models can be quantified in a formal way, which is known as uncertainty analysis. Many approaches has been developed to achieved this quantification, for instance: Monte Carlo method, probabilistic formulations (such as Bayes’ theorem), linear and nonlinear analyses, geostatistical approaches, among many others (Anderson et al., 2015).

### Table 2:5. Examples of aleatory and epistemic uncertainties in hydrologic modeling (adapted from Anderson et al., 2015)

<table>
<thead>
<tr>
<th>Uncertainty from</th>
<th>Aleatory component</th>
<th>Epistemic component</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rainfall observation</td>
<td>Gauge errors, after allowing for consistent bias associated with height, wind speed, etc.</td>
<td>Neglect of, or incorrect corrections for, gauge errors and radar estimates.</td>
</tr>
<tr>
<td>Remote sensing and sensor data</td>
<td>Random error in correction of sensor values to fields of digital numbers</td>
<td>Inappropriate correction algorithms or assumptions about parameters</td>
</tr>
<tr>
<td>Soil-water balance recharge and evapotranspiration estimates</td>
<td>Random measurement errors in meteorological variables</td>
<td>Biases in meteorological variables relative to effective values required to estimate catchment average evapotranspiration</td>
</tr>
<tr>
<td>Aquifer properties</td>
<td>Point observation/measurement errors</td>
<td>Errors associated with lack of knowledge of spatial heterogeneity and preferential flow paths</td>
</tr>
<tr>
<td>Head observations</td>
<td>Point observation/measurement errors</td>
<td>Commensurability errors of simulated equivalent outputs with respect to observed values arising from inappropriate handling of scale effects</td>
</tr>
<tr>
<td>Discharge observations</td>
<td>Fluctuation in stage observations and measurement error in direct discharge observations for rating curve definition</td>
<td>Poor methodology and operator error</td>
</tr>
</tbody>
</table>

Anderson et al., 2015
3. Study Area

The study was conducted in the municipality of Tacherting, a community situated in the northern part of the District of Traunstein in the State of Bavaria, Germany. The area of Tacherting is 50.24 km² with a population of approximately 5500 inhabitants, and the nearest major cities are Salzburg and Munich at 50 and 80 km distance, respectively. Tacherting includes residential and recreational areas, as well as zones covered by forest. Commercial areas and an industrial park are part of the business structure of the community (Gemeinde Tacherting, 2017c, 2017d). In spite of the industrial expansion due to cheap energy supply, the surrounding settlements maintain the character of villages (Doppler, 1982). Figure 3:1 includes a map of the location of the study area.

![Map of the location of the study area](image)

*Figure 3:1. Location of the study area*

The study area is located in the prealpine region, which is limited in the south by the northern edge of the Alps. Tacherting differs from the Alpine region by its lower elevation (Orendt, 2003) at an altitude of 473 m above the sea level (Gemeinde Tacherting, 2017a). The area of interest...

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lies on the left bank of the River Alz and it is determined by the topography of the lower Alz Valley (Unterreitmeier, 2011b). The Figure 3:2 represents the topography of the area of interest, developed based on the dataset issued in the investigation of Keilholz, Kumar, & Disse (2015). It is here possible to observe that the east and the west sides of the study area consist of two hills of approximately 480 and 520 m above the sea level, respectively. These elevations enclose the valley above where the Alz river and the Alz channel flow.

![Topographic map of the study area (in meters a.s.l.)](image)

**Figure 3.2: Topographic map of the study area (in meters a.s.l.)**

### 3.1. Hydrological description

One of the main features of the study area is the Alz River. The Alz borders the eastern edge of the village. It origins in the south from the Chiemsee Lake, the largest lake in Bavaria (Harper, Brierley, Ferguson, & Phillips, 2013), also known as the “the Bavarian Sea” (Stahr & Langenscheidt, 2014). The catchment area of the Alz is at the mouth of the Inn 2,265 km² (Stemmer, 2013) and it falls into the Inn River in the north after 63 km. The Alz flows from southwest to northeast through the District of Traunstein and the District of Altötting, and in this course, the only major tributary is the Traun River, which flows into the Alz at the municipality of Altenmarkt (Wasserwirtschaftsamt Traunstein, 2005).

Unterreitmeier (2011a) states that the hydrology in the Alz is determined by two different types of flood wave. When the Alz begins in the Chiemsee Lake in Seebruck and flows between Seebruck and Altenmarkt in a predominantly natural stream bed, the flood waves are strongly attenuated by the lake retention of the Chiemsee. On the contrary, at the height of Altenmarkt, the Traun river flows into the Alz, and these flood waves from the Traun run very fast and are
characterized by a pronounced peak of runoff. Figure 3:3 shows an overview map of the study area.

As is shown in Figure 3:1, the municipality of Tacherting also includes other hamlets and villages. One of this is Wajon, where one of the power plants of the region was constructed in 1908. The plant is currently producing and the installed capacity is 8 MW (Alzkraftwerke Heider GmbH, 2011). An artificial waterway, the Alz channel, is situated in the west of Wajon, and it was built in order to reroute the water of the Alz to generate electricity through the run-of-river operation. Additionally, Wajon and the lower village of Tacherting are settlements placed in floodplain areas (Unterreitmeier, 2011b). In the years 1991 and 2013, there were building damages due to seepage of groundwater (Disse, Keilholz, & Kumar, 2015).

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8 Map source: Esri Basemap

9 Run-of-river plants are power stations that are built into the actual riverbed, normally to produce energy in low-head plants without any storage (Kaltschmitt, Streicher, & Wiese, 2007).
Regarding the land use, the study place includes areas for agriculture due to the high fertility of the soil, and the advantages for workability, which is favored by both the balanced relief and the soil structure (Doppler & Grottenthaler, 1982). Additionally, permanent pastures and forest coverage can be found immediately at the riverside and next to the water channel. Between the villages and the Alz is a mound, which is covered by shrubs and trees, for protecting the residences from floods. Figure 3:4 shows pictures of the study area.

![Figure 3.4. Pictures of the study area: Alz river (left) and power plant on the Alz channel (right).](image)

3.2. Geological and hydrogeological description

The geological structure of the region have been deeply investigated, linking the stratigraphy to the landscape development (e.g., Doppler, 1980, 1982, 1982; Ebers, Weinberger, & Del-Negro, 1966; Lemcke, 1988; Sidiropoulos, 1980; Traub, 1975). Terrace units are often applied for the classification of stratigraphic divisions of soil (Doppler et al., 2011), which are used to estimate soil characteristics of the study area. Lower terraces of gravel compose the western edge of the area, while the eastern edge is formed by higher terraces of mainly proglacial gravel from the glacier advance phase. The valley is formed by deposits of young floodplains. Stratigraphic units of Tacherting are mapped in Figure 3:5.

![Figure 3.5. Soil units of the study area (from Bayerisches Landesamt für Umwelt, 2017)](image)

Legend
- River or stream
- Deposits of the autochthonous valleys
- Deposits of the younger floodplain
- Deposits of the recent floodplain
- High terraces, thrust gravel and fissure rock
- Lower terraces of gravel
- Gravel of the middle postglacial terrace
- Gravel of the upper postglacial terrace
- Gravel of the lower postglacial terrace
- Gravel of the older late glacial terraces
- Gravel moraine with wall form
- Alluvial fan
- Advancing gravel and younger ceiling gravel
The valley of the Lower Alz was formed mainly during the last two ice ages: the Riss glaciation and the Würm glaciation (Wasserwirtschaftsamt Traunstein, 2005). Consequently, the region is largely composed of gravel deposits derived from melted water pathways of central Alpine glaciers (Doppler et al., 2011). Keilholz et al., (2015) remarks that the soil composition in Tacherting allows a very dynamic groundwater flow and classify two predominant regions: high permeable low-terrace and late-glacial terraced gravel layers (permeability: $5 \times 10^{-3}$ m/s), which may be interspersed with thin layers of sediment (meadow ash), and the area of higher terraces where less permeable layers of paving (permeability: $4 \times 10^{-4}$ m/s). Table 3:1 shows the rough permeability expected in this study.

Table 3:1. Soil type predominant regions (Keilholz et al., 2015)

<table>
<thead>
<tr>
<th>Identified units</th>
<th>Description of the units</th>
<th>Expected permeability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low-terrace and late-glacial terrace of gravel layers</td>
<td>High permeable</td>
<td>$5 \times 10^{-3}$ m/s</td>
</tr>
<tr>
<td>Higher terraces</td>
<td>Less permeable layers</td>
<td>$4 \times 10^{-4}$ m/s</td>
</tr>
</tbody>
</table>

The particular importance of the protection of groundwater for public water supply in Bavaria has been recognized by the public sector, and it includes the attention of the effect of high groundwater levels due to flood events and heavy precipitation, which may temporarily lead to a change in the behaviour of groundwater flow (Bayerisches Landesamt für Umwelt, 2016).

3.3. Climatology

According to the meteorological data from 2008 to 2017 (Agarmeteorologie Bayern, 2017), which is sketched in Figure 3:6, the mean temperature of the region is 9.2 °C, with a monthly mean maximum of 21.3 °C and a monthly mean minimum of 9.2 °C. The warmest temperatures are recorded during the months of June, July and August. On the other hand, December, January and February are the coldest months, often reaching mean temperatures under zero degrees Celsius. As was expected with the temperature, the highest values of radiation and hours of sunshine coincide with the summer; and, during the winter, the mean values of total radiation and the hours of sunshine are the lowest recorded. Finally, the highest values of relative humidity are found from October to January, where is possible to register monthly mean values above 90%.
Figure 3.6: Meteorological data from the weather station of Schönharting (from Agrarmeteorologie Bayern, 2017): a) average temperature per month; b) average wind velocity per month; c) water balance per month; d) average humidity per month; e) total radiation per month; and, f) hours of sunshine per month.
Over the period of ten years (Agrarmeteorologie Bayern, 2017), it is possible to observe annual precipitation patterns. The highest rainfall events occur during the summer and the beginning of autumn. June and July are the months with the heaviest precipitations. The two highest peaks correspond to June 2009 and May 2013, when the total monthly precipitations were higher than 200 mm. Furthermore, during the event of 2013, floods were registered in the lower area of Tacherting and Wajon (cf. Figure 3:7).

![Figure 3:7. Monthly precipitation in the region of Tacherting (from Norwegian Meteorological Institute & Norwegian Broadcasting Corporation, 2017)](image)

For a better understanding, data from a longer period (Norwegian Meteorological Institute & Norwegian Broadcasting Corporation, 2017) is shown in Table 3:2. It shows the monthly average temperature, and the average amount of days with precipitation (when precipitation has surpassed 1 mm per day) per month for the period 1961–1990. As Doppler & Grottenthaler (1982) mention, it is important to consider that the highest monthly temperatures coincide with the heaviest rainfalls in this region.

Table 3:2. Temperature and precipitation per month in Tacherting (from Norwegian Meteorological Institute & Norwegian Broadcasting Corporation, 2017)

<table>
<thead>
<tr>
<th>Month</th>
<th>Average daily temperature</th>
<th>Average amount of days with precipitation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Normal</td>
<td>Warmest</td>
</tr>
<tr>
<td>January</td>
<td>-1.4 °C</td>
<td>1.7 °C</td>
</tr>
<tr>
<td>February</td>
<td>-0.1 °C</td>
<td>4.0 °C</td>
</tr>
<tr>
<td>March</td>
<td>4.1 °C</td>
<td>9.2 °C</td>
</tr>
<tr>
<td>April</td>
<td>7.8 °C</td>
<td>13.2 °C</td>
</tr>
<tr>
<td>May</td>
<td>13.2 °C</td>
<td>18.8 °C</td>
</tr>
<tr>
<td>June</td>
<td>15.9 °C</td>
<td>21.2 °C</td>
</tr>
<tr>
<td>July</td>
<td>17.8 °C</td>
<td>23.5 °C</td>
</tr>
<tr>
<td>August</td>
<td>17.3 °C</td>
<td>23.5 °C</td>
</tr>
<tr>
<td>September</td>
<td>13.3 °C</td>
<td>19.2 °C</td>
</tr>
<tr>
<td>October</td>
<td>8.2 °C</td>
<td>13.3 °C</td>
</tr>
<tr>
<td>November</td>
<td>2.8 °C</td>
<td>6.2 °C</td>
</tr>
<tr>
<td>December</td>
<td>0.0 °C</td>
<td>2.7 °C</td>
</tr>
</tbody>
</table>
3.3.1. Flood events in Tacherting

In the recent years, extreme precipitation events have led to floods in Central Europe, causing serious damage to the economy, and affecting households and communities (Bundesministerium für Verkehr, Bau und Stadtentwicklung, 2013). Particularly, the heavy rainfall at the end of May and the beginning of June 2013 caused great damage in the municipality of Tacherting. The flow of surface water, the rising water levels of the streams and the associated increase in groundwater levels have led to bad conditions (Gemeinde Tacherting, 2017b), especially building damages were registered due to seepage of groundwater (Disse et al., 2015).

Various investigations have been performed to understand the flood events in Tacherting and, also, some projects have been proposed to reduce the associated risk and the negative effects of extreme events in the residential zones (e.g., Disse et al., 2015; Haimerl et al., 2002; Keilholz et al., 2015; Stemmer, 2013; Unterreitmeier, 2011b). Some of the proposed solutions for flood protection are the redesign or relocation of the dike, the installation of pumping stations for draining, the sealing of the bottom of the Alz channel, among others.

The studies of Keilholz et al., (2015) and Disse et al., (2015) examine some possible influences for the rising of groundwater levels such as the weir, the sealing measures on the sewage system, the changes in agricultural use, and the climate change. These investigations include the development of integrated models (linking groundwater and surface water), and the quantification the effect of heavy precipitation and river floods during the event in 2013. They suggest that the impact of the flood event in Tacherting was significantly raised due to the floods in the Alz river, a not only due to the heavy precipitation (cf. Figure 3:9).

Figure 3:8. Pictures of the overflows during the flood event in 2013 the residential zone of Tacherting (left) and Wajon (right) (Disse et al., 2015)
In a previous investigation, Haimerl et al., (2002) analysed the groundwater flow pattern and stated that the groundwater level is regulated by the drainage effect of the Alz undercurrent of the Tacherting’s weir at the north of the village, neglecting the effect on groundwater of water level in the weir. Also, it remarks that a meaningful rising of the groundwater level can be possible if the river stage is above the groundwater level. In fact, the analysis of the data showed that the correlation coefficients between the groundwater level and the outflow of the Alz river are very high.
4. Materials and methods

This study develops a three-dimensional numerical model of the groundwater flow of the valley of Tacherting in order to describe groundwater flow under flood conditions, and evaluate the associated uncertainty due to river boundary conditions. The simulation was performed using MODFLOW-2005 (Harbaugh, 2005) as code for solving the finite-difference model, and Processing Modflow (Chiang, 2011; Simcore Software, 2012) as graphical interface.

4.1. Dataset and data analysis

The starting point of this study is an existing hydrological model of the region (Keilholz et al., 2015), which was developed with the purpose of analyzing the influences on the groundwater levels due to the interaction groundwater-surface water. The model was done using MIKE SHE, a physically based distributed hydrological model, developed by the Danish Hydraulic Institute (DHI) on the basis of the SHE (Système Hydrologique Européen) code (DHI, 2017). This study served as the basis to determine the time-variant hydraulic heads of the aquifer along as the data set for the setup and the calibration of the model. For the hydraulic heads, infiltration distribution and topography (digital elevation model), an adjustment of the data (through linear interpolation of 2D gridded data in MATLAB) was necessary to fit the resolution of the model of this study. The set of data used in this study is summarized in Table 4:1 including the database and the original source of information.

<table>
<thead>
<tr>
<th>Data</th>
<th>Database</th>
<th>Source of information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stream water levels*</td>
<td>Keilholz et al., 2015</td>
<td>WWA Traunstein</td>
</tr>
<tr>
<td>Digital elevation model</td>
<td>Keilholz et al., 2015</td>
<td>Bayerisches Landesamt für Umwelt</td>
</tr>
<tr>
<td>Groundwater levels</td>
<td>Keilholz et al., 2015</td>
<td>Heider Kraftwerke; TU München; WWA Traunstein</td>
</tr>
<tr>
<td>Precipitation</td>
<td>Agrarmeteorologie Bayern</td>
<td>Agrarmeteorologie Bayern</td>
</tr>
<tr>
<td>Geological data</td>
<td>UmweltAtlas Bayern</td>
<td>Bayerisches Landesamt für Umwelt; Doppler, 1982</td>
</tr>
<tr>
<td>Infiltration**</td>
<td>Keilholz et al., 2015</td>
<td>Keilholz et al., 2015</td>
</tr>
<tr>
<td>Time-variant heads**</td>
<td>Keilholz et al., 2015</td>
<td>Keilholz et al., 2015</td>
</tr>
</tbody>
</table>

* It includes river stage and water level in the channel
** Data extracted from the model results of the existing model
4.2. Groundwater flow process modeling

4.2.1. Conceptual model

Although, groundwater models can be roughly divided into physical models and mathematical models, the development of a conceptual model is one of the initial steps in the modeling workflow (Anderson et al., 2015). Conceptual models describe the groundwater flow in the aquifer system, explaining how water enters to the system. They begin as simple conceptions allowing to share the basic knowledge and providing a critical assessment for further insights. Normally, they are represented as sketches, diagrams based on geological cross-sections and flow directions (Rushton, 2003).

A generic conceptual model was done to organize information and represent in a simplified mode the complex nature of the system. The conceptual model was based on the field data and available information from the site. It describes briefly and graphically the groundwater flow system including associated streams, geological characteristics and system boundaries. Additionally, it includes the main components of the water budget. The conceptual model drives the development of the subsequent numerical model, especially for those components referred to

4.2.2. Numerical model

Domain and discretization of the model

The first step for the development of the numerical model of groundwater flow is the definition of the domain and the spatial and temporal discretization. Spatially, the system was subdivided, vertically and horizontally, into a finite difference grid of rectangular blocks or cells, which consists of 8 layers (variable dimensions), 220 rows (5 m each one) and 300 columns (5 m each one). Thus, the extension of the modeled area is 1500 m from west to east, and 1100 m form south to north. The model domain is delineated based on the surface topography and local physical boundaries which are reviewed in the conceptual model. Time-dependent groundwater heads are defined along the perimeter. Cells out of the perimeter were defined as inactive cells. The model grid encompasses 528000 grid cells, of which 358144 are actively simulated. The discretization in time is established to aim a transient simulation since the model is assumed to be time dependent. Therefore, a period of 37 days is divided into 148 stress periods of 6 hours of length, involving the period from 25th of May, 2013 (00:00:00) until 30th of June, 2013 (18:00:00). Each stress period is configured with only one time step. The characteristics of the model domain and the extension are summarized in Table 4:2 and Table 4:3, respectively.
The elevation of the top of layer 1 is defined according to the topography of the area. To adjust the resolution of the topographical dataset (10 m²) for the discretization of the model (5 m²), an interpolation of 2D gridded data, based on linear interpolation, was performed in MATLAB. For layer 2, the elevation of the layer top is defined considering the lowest elevation of the top of layer 1, to avoid conflicts between the elevations of the top and bottom of the layers. From layer 2 to layer 8, the thickness is four meters each one, and only layer 1 has a variable thickness according to the physical shape of the surface. The bottom of the aquifer (at the bottom of layer 8) is elevated at 435 m a.s.l. It is important to mention that the elevation of the confining layers vary to adjust them with the interpretation of the conceptual model.
Setup of model parameters

The setup of the model was done by specifying the aquifer properties through the corresponding terms. These properties are the horizontal hydraulic conductivity (HK), vertical hydraulic conductivity (VK), specific yield (SY), and specific storage (SS). The initial set of parameters were adjusted by consideration of representative values for a given hydrologic property based on available field data and site conditions, as well as accepted limits reported in the literature. The parameters were adjusted until the model simulated predevelopment conditions within acceptable tolerances. Three soil types were identified in the area: SA (sand and gravels), SB (sand, gravels and alluvial deposits), and SC (gravels, sand and rocks). The specified vertical and horizontal hydraulic conductivity varies according to the type of soil.

Heterogeneous hydraulic conductivity fields generation

Even though the hydraulic properties of the system are assumed to be homogeneous within each cell, the horizontal and vertical hydraulic conductivities were considered heterogeneous among the cells, and they are also subdivided according to the soil types. Hence, heterogeneous fields for both horizontal and vertical hydraulic conductivity were applied in each layer for stochastic modeling, using the Field Generator of PMWIN (Chiang, 2011; Simcore Software, 2012) to create log-normal correlated distributions of the hydraulic conductivity. The subsequent realizations were randomly assigned in MATLAB, and the final fields are the result of the combination of these random fields considering the soil types of each layer.

Mathematical representation of boundaries and flow packages

The mathematical representation of boundaries can be done in more than one way, depending on the specified statement. At the boundaries of the domain, one can specify the dependent variable (head), or the derivative of the dependent variable (flux). The model includes head dependent flow boundaries, Cauchy boundary conditions, for the heads of the aquifer as well as for the streams.

Boundary conditions of groundwater levels were defined according to the previous model developed by Keilholz et al. (2015). Figure 4:2 helps to exemplify how the specified heads were extracted from the existing regional model, and Figure 4:3 shows the comparison between observed and calculated heads from the reported results. These boundary conditions were specified with the time-variant specified head (CDH) package in order to observe and introduce in the numerical model the fluctuations in groundwater levels due to the changes between stress periods of specified hydraulic heads. River package (RIV) was used to include the effects of flow between the river and the groundwater regime. Geostatistical procedure that generates an estimated surface from a scattered set of points. The stages of both river and channel were
separately interpolated to estimate the surface from the original set of scatter points. The interpolation was done through the geostatistical procedure of the Kriging tool of ArcGIS (Esri, 2017). The resulting raster files were transformed in ASCII files to be used as inputs in Processing Modflow.

Figure 4.2. Regional hydraulic heads from the existing model (from Keilholz et al., 2015)

Figure 4.3. Hydraulic heads from existing model (from Keilholz et al., 2015): a) B1 and b) B3
4.2.3. Calibration and parameter estimation

Calibration targets are those values which are compared with the simulated values during the matching to describe the model fit. For this study, these values are obtained from three monitoring wells (cf. Table 4:4). These monitoring wells were selected because they presented information during the evaluated period with the required interval of time in accordance with the time discretization of the numerical model.

**Table 4:4. Monitoring wells location**

<table>
<thead>
<tr>
<th>Monitoring well</th>
<th>Coordinates*</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>North</td>
<td>East</td>
</tr>
<tr>
<td>Alzpitz</td>
<td>4543130</td>
<td>5326369</td>
</tr>
<tr>
<td>B1</td>
<td>4542820</td>
<td>5326060</td>
</tr>
<tr>
<td>B3</td>
<td>4543140</td>
<td>5326520</td>
</tr>
</tbody>
</table>

The model was calibrated adjusting the hydrologic properties combining manual matching and the regularized inversion process of the parameter estimation code PEST (Doherty, 2010b, 2010a). To adjust and represent the parameters, additional to the soil classification, a supplementary zonation for the riverbed conductance was done, based on the different condition of the natural stream, (the Alz river), and the artificial channel (the Alz channel). Therefore, the parameters included in the calibration were: \(HK_{SA}, HK_{SB}, \) and \(HK_{SC}\) (horizontal hydraulic conductivity according to the soil classification); \(VK_{SA}, VK_{SB}, \) and \(VK_{SC}\) (vertical hydraulic conductivities according to the soil classification); \(SS\) (specific storage); \(SY\) (specific yield); \(RC_R\) (riverbed conductance); and, \(RC_{C1}\) and \(RC_{C2}\) (streambed conductance of the channel).

To quantify the sensitivity of the model parameters a sensitivity analysis was performed with respect to the calibration targets. The method was the composite parameter sensitivities using PEST. This method is useful to identify those parameters which may be degrading the performance of the parameter estimation process because of the lack of sensitivity model outcomes (Chiang, 2011).

4.3. Uncertainty analysis

The uncertainty analysis consists in a basic uncertainty analysis through scenario modeling to produce a group of results that defines a representative envelope of uncertainty around the simulation. The scenarios are executed as a forward run and the results are evaluated through linear regression. In addition, the possible sources of uncertainty in the numerical model are discussed in Chapter 6 to incorporate a qualitative evaluation into the analysis.
The scenarios are simulated using different parameter sets for the river and channel. These proposed scenarios of uncertainty are considered plausible for the purpose of study. All the previous calibrated parameters were retained except for those related to the stream properties: river stage and riverbed conductance. It is important to clarify that these evaluations were developed not only for the parameters of the Alz river but also for the channel, since it was assumed to be hydrologically connected to the aquifer.

The scenarios related to the uncertainty on the river and channel stage were executed considering variations of ±15% in the water level. This variation is calculated as percentage of the height between the water level of the stream and the top of the streambed. On the other hand, the scenarios for both channel bed conductance and riverbed conductance were simulated considering variations of ±50%. The simulations are run independently to evaluate the uncertainty of these parameters separately. This means that the simulation of bed conductance and stage were not performed simultaneously. The evaluation of the uncertainty includes the comparison to the different scenarios and the base model results through linear regression. For this purpose, three extra simulation scenarios of uncertainty were performed varying riverbed conductance in ±75%, and +110%. This also allows to understand how the relative change in each scenario influence the model outputs.

4.4. Solute transport simulations

The study includes the evaluation of a hypothetical scenario of solute transport under the extreme conditions of the selected. The constant-density transport simulation was performed to recognize, under flood conditions, the behavior of a hypothetical solute, Solute A, and its produced plume. The simulation was performed using as transport solution technique the modular three-dimensional transport model MT3DMS (C. Zheng & Wang, 1999). The theoretical approach considered that changes in concentration were caused for advective, dispersive, and diffusive transport and the assumptions do not include any kinetic reactions or sorption.

Therefore, the scenario is based on the instantaneous injection of the Solute A, placed between the monitoring wells B1 and Alzpitz (layer 1, row 36, column 136), at an initial concentration of 12500 µm of Solute A. It is placed in one cell in the upper layer, in order to simulate the transport of a solute discharged near to the surface. The simulation started, in unique event, in the stress period one and the concentration distributions were calculated after 37 days. The solution scheme implemented for solving the advective transport was an Eulerian-Lagrangian method known as Method of Characteristics (MOC). Table 4:5 indicates the model parameters that were assumed, based on literature review (Davis, 2003), for the solute transport modeling.
Table 4.5: Model parameters for solute transport modeling

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial concentration $C_0$</td>
<td>µg/m³</td>
<td>15000.00</td>
</tr>
<tr>
<td>Effective molecular diffusion coefficient $D^*$</td>
<td>m²/s</td>
<td>0.00</td>
</tr>
<tr>
<td>Longitudinal dispersivity $\alpha_L$</td>
<td>m</td>
<td>1.70</td>
</tr>
<tr>
<td>Transverse dispersivity (horizontal and vertical) $\alpha_{TH}, \alpha_{TV}$</td>
<td>m</td>
<td>0.29</td>
</tr>
<tr>
<td>Distribution coefficient $K_d$</td>
<td>m³</td>
<td>0.000125</td>
</tr>
<tr>
<td>Porosity $n$</td>
<td>-</td>
<td>0.26</td>
</tr>
<tr>
<td>Bulk density $\rho$</td>
<td>kg/m³</td>
<td>2000.00</td>
</tr>
</tbody>
</table>

Three points in the model were selected for the evaluation of the spatial distribution of the concentration, as is shown in Figure 4.4.

The USGS particle-tracking code MODPATH (Pollock, 1994) was used to generate the advective pathlines of water particle and their associated travel time based on MODFLOW simulations. The MODPATH code was used in forward-tracking mode to evaluate flow paths from areas near to the river and to the channel, as well as in backtracking mode to evaluate further areas where human settlements are placed. Finally, the numerical groundwater model provides information about the flows through the different faces of the cells that the model comprises. The flows from the cells were used to generate two-dimensional velocity fields, which were plotted and illustrate magnitude and direction of the instantaneous velocity vectors.
5. Results

5.1. Conceptual model

The current section presents the generic conceptual model for the understanding of the hydrogeological conditions of the study area. The conceptual model drives the rest of the modeling process, providing the fundamental framework for designing the numerical model. Therefore, the results represented in the conceptual model are analyzed in this section and they are represented in Figure 5.1.

Figure 5.1. Generic conceptual model of the study area
The hydraulic properties of the aquifer are intimately related with the topography of the area. The local aquifer is not only fed by the flows coming from the south, but also from superficial and sub-superficial flows from the higher hills at the east and west.

Regarding to the lithology of the area, deeper layers of the Tertiary consist of clays and marls with sand and gravel inclusions, which confine the bottom of the aquifer, while the upper and younger layers are composed by sand and gravel. Additionally, it is possible to observe alluvial deposit which includes river clays. The confining layer is expected between 430 and 450 m a.s.l., approximately. The stratigraphy of the region presents significant differences in the heights of the confining layer at different locations, which are considered in the definition of the numerical model. As is observable in the Figure 5:1., the confining layer in the area immediately below the river are around 20 m shallower.

The region formed by sand and gravels has the permeability conditions required for groundwater storage and dynamic flow. In Figure 5:1, the interaction between the river and the aquifer are sketched. It is expected during the analyzed period that the Alz River and the artificial channel act as influent stream for the aquifer, because the stages of the river and the channel are higher than the phreatic level of the aquifer. The aquifer flow is expected to run from south to north due to the hydraulic conditions and the gradient caused by topographical characteristics.

Three units are differentiated in the area according to the geological characteristics: (1) SA is the region formed by sand and gravels, (2) SB is the region immediately below the river that is formed by sand and gravels but also for the younger alluvial deposits; and, (3) SC is the western formations in the higher terraces formed mainly by gravels, which alternate with sand and rocks.

5.2. Groundwater flow model

5.2.1. Simulated hydraulic heads

The results of the model presented in this section correspond to those after the calibration process. Figure 5:2 represents graphically the comparison between the calculated phreatic level and the observed in the monitoring wells along during the period selected for the study. Figure 5:3 shows a contour map of the calculated hydraulic heads at different times to illustrate the distribution of the simulated heads and their temporary changes, particularly during the flood event. A comparison of calculated and observed heads is shown in the scatter diagram of Figure 5:4. Additionally, the head distribution over the different layers of the domain are shown in F5, where different instants of the simulation were chosen to illustrate the variations.
Figure 5.2: Head-time curves: a) Alzpit, b) B1, and c) B3
Figure 5.3. Contour map of simulated hydraulic heads (layer 1)
5.2.2. Evaluation of the calibrated model

The results of the calibration were evaluated qualitatively and quantitatively based on the calibration targets. The results of the quantitatively evaluation are summarized in Table 5:1. These statistical measures quantify the error considering the distribution of the residuals rather than represent a definition of the accuracy of the model.

Table 5:1. Results of the statistical evaluation of the calibrated model

<table>
<thead>
<tr>
<th>Expected values</th>
<th>Alzpitz</th>
<th>B1</th>
<th>B3</th>
<th>Overall</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variance</td>
<td>0.023</td>
<td>0.072</td>
<td>0.015</td>
<td>0.036</td>
</tr>
<tr>
<td>Mean error</td>
<td>-0.001</td>
<td>0.083</td>
<td>0.015</td>
<td>0.033</td>
</tr>
<tr>
<td>Mean absolute error</td>
<td>0.116</td>
<td>0.238</td>
<td>0.105</td>
<td>0.153</td>
</tr>
<tr>
<td>Pearson correlation coefficient</td>
<td>0.962</td>
<td>0.880</td>
<td>0.951</td>
<td>0.960</td>
</tr>
<tr>
<td>Pearson’s chi squared</td>
<td>0.007</td>
<td>0.023</td>
<td>0.005</td>
<td>0.035</td>
</tr>
</tbody>
</table>

Simulated water budget

According to the simulated water budget, the mean flow into the domain for the period before the flood (20 first stress periods from May 25th to June 30th) is 2.60 m³/s, whereas during the
peak of the flood it is more than 4,83 m$^3$/s. In average the flow into the system during the whole simulated time is 2,69 m$^3$/s. The water budget discrepancy was -0,013.

Figure 5.5. Water budget inputs and outputs

Estimated hydraulic parameters and sensitivity analysis

The estimated parameter and their results from the sensitivity analysis are shown in Table 5.2. Sensitivities of the parameters were extracted from the records file of PEST, which calculated overall sensitivity of each parameter according to the last and final estimation.

Table 5.2. Final model parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>HKsa (mean)</td>
<td>m/s</td>
<td>7.4131×10^{-01}</td>
<td>8.450120×10^{-09}</td>
</tr>
<tr>
<td>HKsb (mean)</td>
<td>m/s</td>
<td>5.8670×10^{-01}</td>
<td>5.888182×10^{-08}</td>
</tr>
<tr>
<td>HKsc (mean)</td>
<td>m/s</td>
<td>1.2161×10^{-02}</td>
<td>1.581157×10^{-07}</td>
</tr>
<tr>
<td>VKsa (mean)</td>
<td>m/s</td>
<td>2.2128×10^{-04}</td>
<td>2.362763×10^{-05}</td>
</tr>
<tr>
<td>VKsb (mean)</td>
<td>m/s</td>
<td>7.5300×10^{-04}</td>
<td>8.170012×10^{-05}</td>
</tr>
<tr>
<td>VKsc (mean)</td>
<td>m/s</td>
<td>8.1611×10^{-04}</td>
<td>6.897383×10^{-05}</td>
</tr>
<tr>
<td>SS</td>
<td>m-1</td>
<td>3.6625×10^{-04}</td>
<td>5.766557×10^{-04}</td>
</tr>
<tr>
<td>EP</td>
<td>-</td>
<td>0.26</td>
<td>-</td>
</tr>
<tr>
<td>SY</td>
<td>-</td>
<td>0.18</td>
<td>2.465813×10^{-04}</td>
</tr>
<tr>
<td>RCr</td>
<td>m$^2$/s</td>
<td>3.8520×10^{-04}</td>
<td>6.175499×10^{-04}</td>
</tr>
<tr>
<td>RCC1</td>
<td>m$^2$/s</td>
<td>3.4873×10^{-04}</td>
<td>5.912551×10^{-04}</td>
</tr>
<tr>
<td>RCC2</td>
<td>m$^2$/s</td>
<td>6.2461×10^{-04}</td>
<td>8.130682×10^{-04}</td>
</tr>
</tbody>
</table>
Figure 5.6: Graphical representation of the composite sensitivity of the model parameters

Heterogeneous hydraulic conductivity fields

As substantial part of the stochastic modeling, the results of the random generation of hydraulic fields are shown in this section. Table 5.3 show the settings used for the generation of the fields. To evaluate the distribution of the hydraulic conductivity, the horizontal and vertical fields are plotted in Figure 5.7 and Figure 5.8, respectively.

Table 5.3: Conditions for generating heterogeneously distributed hydraulic conductivity fields

<table>
<thead>
<tr>
<th>Soil type</th>
<th>Number of realization</th>
<th>Mean value (log₁₀)</th>
<th>Standard deviation (log₁₀)</th>
<th>Correlation length along rows and columns</th>
</tr>
</thead>
<tbody>
<tr>
<td>SA</td>
<td>HK₆₈A</td>
<td>24</td>
<td>-2,1300</td>
<td>0,5</td>
</tr>
<tr>
<td></td>
<td>HK₆₈B</td>
<td>24</td>
<td>-3,6550</td>
<td>0,5</td>
</tr>
<tr>
<td>SB</td>
<td>HK₆₈B</td>
<td>24</td>
<td>-2,2315</td>
<td>0,5</td>
</tr>
<tr>
<td></td>
<td>VK₆₈B</td>
<td>24</td>
<td>-3,1232</td>
<td>0,5</td>
</tr>
<tr>
<td>SC</td>
<td>HK₆₈C</td>
<td>24</td>
<td>-1,9150</td>
<td>0,5</td>
</tr>
<tr>
<td></td>
<td>VK₆₈C</td>
<td>24</td>
<td>-2,2065</td>
<td>0,5</td>
</tr>
</tbody>
</table>
5.3. Uncertainty analysis

Four scenarios of uncertainty were assumed for simulating the groundwater flow and the solute transport. The results of these simulations are shown in Figure 5:9. Additionally, as part of the evaluation of the uncertainty in river boundaries, different scenarios of uncertainty were correlated with the results of the base model through a linear regression (cf. Figure 5:10).
Figure 5.9. Simulated uncertainty scenarios: a) Alzpitz, b) B1, and c) B3
Figure 5:10. Linear regression of hydraulic heads from uncertainty scenarios with respect to base model results: a) Alzpitz, b) B1, and c) B3
5.4. Solute transport simulation

The concentration values were illustrated to observe the spatial distribution of both the transport of the solute and the change in the concentration according to the results of the base model, as well as the proposed scenarios. Additionally, the change in concentration in the three observation points are plotted in Figure 5:16. Notice that, in order to visualize the changes, the plots a) and b) have been graphed as logarithmic function and by normalization, respectively. The normalized values are defined from a distribution characterized by mean and standard deviation.

*Figure 5:11. Spatial representation of solute concentration in layer 1 (base model simulation)*
Figure 5:12. Spatial representation of solute transport in layer 1 (uncertainty scenario +15%)

Figure 5:13. Spatial representation of solute transport in layer 1 (uncertainty scenario -15%)
Figure 5.14. Spatial representation of solute transport in layer 1 (uncertainty scenario +50%)

Figure 5.15. Spatial representation of solute transport in layer 1 (uncertainty scenario -50%)
Figure 5.16. Change in concentrations for the different simulated scenarios: a) OB_1, b) OB_2 and OB_3
5.5. Velocity fields and particle tracking simulations

5.5.1. Forward-tracking

In Figure 5:17, the forward particle-tracking is shown. Three recreations considering the conditions at the different phases of the flood event are sketched. This means, the condition of the specified period were retained and the particle tracking was run to see the flow path during 37 days just under the conditions of that time step. Notice that the arrows represent a time mark of an elapsed time of 4 days. The particles are initially located in the first layer close to the river boundary cells.

![Figure 5:17. Forward particle tracking of particle located close to the streams](image)

*Figure 5:17. Forward particle tracking of particle located close to the streams*
5.5.2. Backward-tracking

The backward particle tracking is shown in Figure 5:18. The particles were spatially distributed in residential areas where flood damages were reported. As well as in the forward-tracking, the arrows represent a time mark of an elapsed time of 4 days and the path are simulated only under the conditions of one time step.

![Backward particle tracking of particles located in residential areas](image)

**Figure 5:18. Backward particle tracking of particles located in residential areas**

5.5.3. Velocity field

The velocity fields of the simulated base model at different time steps are plot in Figure 5:19 to represent the changes in velocity according to the phase of the flood event. Figure 5:20 zooms the central region were the river and channel converge, and adds in the description the direction of the flow at the different stages of the flood. In this section, Figure 5:21 is added to visualize the changes in both modeled and observed hydraulic gradients along the simulation time.
Figure 5:19. Velocity fields of different stress periods of the base model (layer 1)
Figure 5:20. Velocity fields and flow direction of the base model (layer 1)
Figure 5.21. Hydraulic gradient between Alzpitz and B3 during the simulation period
6. Discussion

This study first provides a generic conceptual model (cf. Figure 5:1) that presumes very dynamic groundwater flow due to the soil composition. The medium is pervious and hydraulically conductive, because it is mainly composed by gravels and sand, which naturally represent good conditions for allowing groundwater flow. The aquifer is hydraulically connected with both the Alz river and the Alz channel. The water budget gives evidence of the interconnection between the aquifer and the streams. The aquifer is charged not only by infiltrated water from precipitation but also by the river leakage (cf. Figure 5:5). During the modeled period, the Alz river and the channel only act as influent streams contributing water to the aquifer.

The base model fit involved the determination of the magnitude of the residuals and weighted residuals. Analyzing the graphic of the model fit (cf. Figure 5:4) and the related statistics (cf. Table 5:1) the simulated heads were within the calibration objectives. The results of the measures of the overall model fit suggest that the base model is reliable. The monitoring wells closer to the streams (Alzpitz and B3) present better fit statistic results (cf. Figure 5:2a and Figure 5:2c) than the monitoring well B1 (cf. Figure 5:2b). Monitoring well B1 is located at approximately 150 m from the time-variant specified head boundary. This could be the reason for the difficulty for calibrating this point. Aware of the obstacle that this could signify, I decided to keep the spatial location of the boundaries based on the topography and soil conditions of the area, since the main interest of the model was to evaluate the effect of the river boundary conditions.

As shown in Figure 5:3, during the peak of the flood event (stress period 36) the hydraulic head highly increases, particularly in the areas immediate close to the river and the channel. Thus, it is presumably that the raising of groundwater levels are highly influenced by the overflow and high stage of the river, especially in the vicinity of the river. This consequently suggests that the impacts of the flood event in 2013 were significantly raised due to the flood of the streams and the exerted pressure from the water level. This finding would verify one of the conclusions from previous studies (Keilholz et al., 2015), where they suggested that the impact of the flood event was not only due to the heavy precipitation. On the other hand, from stress period 76 to stress period 148 in Figure 5:3 the simulated hydraulic heads slowly decrease, the influence of the streams decline, and it is vaguely noticeable.

As shown in Figure 5:6, not all the calibration parameters were equally valuable for improving the model fit and this is supported by the composite sensitivity analysis results (Table). The following sensitive parameters highly affect the model outputs: horizontal hydraulic conductivity
of soil SA and SB (HK_{SA} and HK_{SB}), and riverbed and streambed (channel) conductance (RC_{R} and RC_{C2}). As expected, the heterogeneous horizontal hydraulic conductivity (HK_{SA} and HK_{SB}) has a strong influence on the groundwater flow. To get a better representation of the heterogeneity of the porous medium, I used spatially-correlated random fields for stochastic modelling. The field generation was based on the previously estimated value of the hydraulic conductivity, which was used as mean value (cf. Table 5:3) considering the different types of soil for the construction of these fields (cf. Figure 5:7 and Figure 5:8). Furthermore, riverbed (RC_{R}) and channel bed conductance (RC_{C1} and RC_{C2}) affect the model outputs and the calibration of the model. In fact, the riverbed and the channel streambed have very different conductance, and this was also easily observable during the calibration process. To get the calibration targets, the conductance in the streambed of the channel have to be differentiated for one order of magnitude higher than the riverbed conductance. This is conceivably attributable to the different configurations of the streams. On one hand, the Alz river is a natural stream with an alluvial sediment formation underneath. On the other hand, the Alz channel is an artificial channel formed by more pervious material in the streambed.

In the proposed scenarios of uncertainty, it is observable a greater effect in Figure 5:9a and Figure 5:9c, whereas in Figure 5:9b the effects highly decrease due to the distance where the monitoring well B1 is located. This indicates that the effect of the boundary conditions is dependent of the distance of the evaluation, reducing the influence of the river boundary conditions when the distance is greater. However, it is important to notice that a small increase in stress period 127 in monitoring well B1 can be slightly influenced due to the river conditions, because, as can be seen in the water budget (cf. Figure 5:5), the infiltration does not increase at that specific time. Moreover, the overestimation scenarios reach the high values of the peak of the event that are frequently not well-described for the numerical models (cf. Figure 5:9a and Figure 5:9c).

A first insight of the uncertainty in river boundary condition is the related to the measurement errors that propagates uncertainty to calibration parameters. During floods, this uncertainty is frequently greater due to the conditions beyond control. Measurement devices have a limited capacity measuring rapidly changing stage. For instance, peak discharges are not accurate described and often require indirect measurements or adjustment methods to described flood wave velocity. Nevertheless, measurement error is not the only one component of the uncertainty in the model related to river. Parameter simplifications also contributes to the model uncertainty. Particularly, we find uncertainty in the stream stage due to interpolation for the spatial distribution of the water level in the cells, and also it is observable when we assume a homogeneous conductance on the streambed. There is an inherent uncertainty in the riverbed conductance estimation, because the models often assume that it is homogeneous along the river,
although it is heterogeneous in the reality. If we consider that the hydraulic conductivity ranges over several orders of magnitude, whereas the specific yield varies mainly within one order of magnitude, there is inherently more uncertainty in values of hydraulic conductivity. In particular, this could be a major concern in study cases where the influence of the streams is relatively high due to the hydrogeological properties of the area. Furthermore, when we consider the riverbed conductance as a parameter in our models, we are also evaluating the width of the riverbed and the composition of the riverbed material, which are also essentially inaccurate, and their estimations are complex. The description of this riverbed conductance could be addressed through a stochastic approach to evaluate quantitatively the effects of spatial variability, unmodeled heterogeneity and data uncertainty. In stochastic modeling, uncertainty due to unknown spatial variability of the model parameters is addressed directly by assuming that the parameters are random variables.

Figure 5:10 relates the uncertainties of the stream stages and the riverbed conductance. In Figure 5:10a, we can assume that to reach or calibrate the uncertainty of −15% percent in the stage, the riverbed conductance needs to vary around −75%, in those monitoring wells close to the streams. On the other hand, it is not plausible to reach an uncertainty of +15% in the stream stage calibrating the riverbed conductance. This may also suggest that an underestimation of the riverbed conductance exposes the model to a large range of error. But also, considering that the peaks of the extreme events are the most difficult to be measured in the field and simulated in the numerical model, this situation reflects a great limitation of numerical simulation of extreme flood events. Particularly important is to identify in Figure 5:10a, the variations at the highest values, which are the values at the peak of the flood event. Considering not only that the model misfits are mainly produced during the peak of the events, but also the uncertainty is higher, this describes the weakness of the numerical simulations to clearly represents the peak of an extreme flood event.

The objective of the transport modelling was to observe the effects of the uncertainty of the river boundary conditions in the simulation. It is possible to observe in Figure 5:11 how the concentration varies spatially due to the advective and dispersive transport. As expected, the spreading of the solute is greater in the scenarios that overestimate the results of the base model. Increments in the water level of the streams induce pressure into the aquifer and, consequently, the movement of the solute in the aquifer at different ranges. Besides the solute concentration decreases rapidly, the plume does not travel considerably from the initial location. The plumes of solute move 15 to 20 m from the initial location. The particle tracking gives evidence of one of the reasons why this occurs. As can be seen in Figure 5:17 and Figure 5:18, the advective transport considerably decreases after the peak of the flood (from stress period 40) and the velocity is significantly lower (cf. Figure 5:19). To evaluate this, I decided to plot the hydraulic
gradient along the simulation period to observe the changes in the gradient, which directly affect the specific discharge of the medium (cf. Figure 5:21). As is observed, the gradient decreases after the peak, even to lower values than at the beginning of the simulation period, and, consequently, the specific discharge also decreases, and the advective movement of the particles slows down.

Furthermore, it is necessary to consider the vertical transport through the different layers. Under flood conditions, the particles move downwards to the lower layers of the domain due to the exerted pressure of the overflow, and this is detected in the particle (cf. Figure 5:17). During the simulation under the conditions of the peak of the flood event (cf. Figure 5:17b), the particles travel downwards through the lower layers and, they travel larger distances from the initial location due to advective transport than the particles under normal conditions (cf. Figure 5:17a). Finally, during the rising flood stage, a reverse motion of the groundwater flow is observed in the velocity field plot (cf. Figure 5:20). These changes in direction of groundwater flow can be caused by the contribution of surface water into the groundwater system at times of high surface-water stages, which are driven by the variations in climate. The water level of the river and the stream can be the two strong hydraulic forces producing this change in the aquifer flow in the zone of Wajon.
7. Conclusions

A three-dimensional numerical model was created to describe the groundwater flow in the aquifer of the valley, and transport simulations were performed to evaluate the solute transport under extreme conditions. In addition, the uncertainty in river boundary conditions was analyzed through a basic uncertainty analysis through scenario modelling considering the stage and the conductance of both the Alz river and the Alz channel. The performed simulations help me to gain knowledge about the temporal and spatial variability of the groundwater flow during the flood event. In addition, uncertainty and sensitivity analysis provided information about the impact of the different variables and tested the model in the presence of uncertainty. The base model accurately represents the conditions of the aquifer during the simulation period, especially in the northcentral area of the domain, where the model fits with the calibration targets.

The model and the solute transport simulations denote the existence of strong interconnection between the aquifer and the streams, which vary depending on the phase of the flood event. The influence of the flood event in the aquifer is particularly noticeable during the higher stages of the flood event and in areas near to the streams. Summing up the conditions of both the river and the channel affect the groundwater flow velocity and direction and this is reflected in the advective transport of the solute. In addition, higher stages during floods and overflow exerted pressure inducing the movement downwards of the particles to the lower layers of the domain.

I conclude that the river boundary conditions in the model control the aquifer responses in the proximities of the streams and that the relative importance of uncertainties in the river boundary conditions is dependent on the distance of the reach of interest and the simulation period of interest. To evaluate these responses and their temporal variation it is necessary to evaluate the flood event before, during and after the peak of the event. As this study demonstrate, the aquifer behavior can widely vary from one of these phases to the next one. This conclusion also reinforces the necessity of enhancing the analysis of uncertainties of river boundary conditions, since the numerical model could not represent the total magnitude of the peak event, the variations can be even larger.

Uncertainty due to river boundary conditions is fundamentally related to measurement errors and parameter simplifications. The uncertainty of these conditions can increase during extreme
events due to the limitations of measurement techniques. Therefore, uncertainty becomes particularly important during extreme events, where the adequacy of numerical models is also challenged, and their forecasting capacity can be questioned. Especially for knowing fate and transport of solutes, the uncertainties due to river boundary conditions should not be neglected beforehand in an uncertainty analysis. In this study, the evaluation of scenarios relies on two components: the stream stage and the streambed conductance. We can intuitively assume a higher importance to the uncertainties if stream stages; however, this study advocates the necessity of evaluate them objectively due to the wide range where the streambed conductance can vary. This research suggests that erroneous assumptions in the riverbed conductance may produce important errors in our model outputs, and this certainly deserves further analysis. Furthermore, it is recommended to make an inventory of the uncertainties involved, quantify them, and estimate their relative effect on the model output. It is necessary to interpret this uncertainty for judging the adequacy of the model results. Certainly, the relative importance and utility of this evaluation will rely on temporal and spatial conditions, the hydrogeological characteristics of the evaluated system, and, of course, the practical objective of the model.

When the hydrogeological properties of the system allow a dynamic subsurface flow, as in the study case of Tacherting, it is required to ponder the estimation of the aquifer-stream interrelationships. The aquifer in the Alz valley is very dynamic, allowing not only horizontal but also vertical groundwater flow. Moreover, both the Alz river and the Alz channel are hydrologically connected to the aquifer. The different results that have discussed in this study may support future research of the floods in the valley of Tacherting.

For further investigations, it is recommended to test the model during longer periods of time through for a quantitative validation of the model. I also suggest carrying out field campaigns for improving the accuracy of the hydrogeological properties of the area, especially those related to soil composition. Future challenges for this study case include: refining of the model for describing with more precision the interaction river-aquifer; applying different methods to analyze the uncertainty of the river boundaries; collecting more data to describe the flood event of the area; applying more rigorous statistical methodology for quantifying uncertainty through inferential statistics and Monte Carlo methods; and, testing and conceptualizing of applied methods for evaluating the uncertainty during extreme conditions, as innovative methods in the groundwater modelling field.
8. References


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