Cross-scale hydraulic characterization of a major karst and alluvial aquifer system for drinking water supply

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ABSTRACT

Groundwater is the most important resource for drinking water supply in Germany, but also in many other countries worldwide. Draughts, heavy rainfall and increasing evapotranspiration, phenomena that are intensified by climate change, reduce the available amount of groundwater. In combination with an increasing demand caused by higher temperatures, maintaining a functioning and sustainable water supply is one of the most important and urgent tasks water suppliers currently have to face. In order to develop and implement necessary adaptations, a good knowledge of groundwater resources is necessary, which can only be achieved by detailed investigations of the catchment areas and aquifers.

In this thesis, the complex karst and alluvial aquifer system in the groundwater protection area Donauried-Hürbe is investigated. It includes large parts of the eastern Swabian Alb and the Danube valley in Baden-Württemberg and was established for the more than 200 extraction wells in the Donauried that are operated by the Zweckverband Landeswasserversorgung. The extracted water contributes to the drinking water supply of around 3 million people in southern Germany, including the Stuttgart metropolitan region. The aim of this thesis is a multi-scale characterization of the extraction wells' catchment area, especially with regard to the inflow towards the Danube valley. While single-borehole dilution tests (SBDTs) are used to investigate the small scale, the large scale is examined with a regional multi-tracer test.

SBDTs are a tracer-based method for characterizing groundwater monitoring wells and boreholes. They are applicable in all aquifer types – especially interesting are heterogeneous karst or fractured aquifers – and can be conducted as uniform injections or point injections. Uniform injections aim to achieve a homogeneous tracer concentration throughout the entire saturated length of a borehole and generate information about major inflow and outflow horizons. Also, in the absence of vertical flow, horizontal filtration velocities can be calculated. The most common method for uniform injections uses a hosepipe to inject a tracer solution.

In the first study, a simplified method for uniform injections under natural flow conditions is developed, evaluated and compared to the widely used hosepipe method. The new method uses a permeable injection bag (PIB) to achieve a close-to-uniform tracer distribution within the saturated zone. The PIB method is used for several tests in the laboratory, as well as for SBDTs in multiple wells in the study area, to allow for a substantiated evaluation. Repeated tests in selected wells are used to assess the reproducibility of the new PIB method. Furthermore, two different calculation methods, based on linear regression and the one-dimensional advection-dispersion equation, are used to calculate apparent horizontal filtration velocities. The obtained results prove that the PIB method delivers valuable and reproducible results for the tested groundwater monitoring wells. Also, it is highly flexible regarding well depth, requires less equipment than comparable methods and can easily be conducted by a single person.

The second study presents a new probe for point-injection SBDTs that is developed and tested during this thesis. By injecting tracer into a specific depth interval, a detailed investigation of the flow processes in this particular depth can be obtained. Also, while uniform injections tend to deliver ambiguous results on vertical flow that often occurs in karst or fractured aquifers, point injections are especially suitable to detect natural vertical flow. Knowledge of vertical groundwater flow is important to understand hydraulic processes in complex aquifers. The developed injection probe is designed to release up to 500 mL of tracer solution into a specific depth without disturbing natural groundwater flow during the injection process. It consists of a hollow cylinder equipped with an opening mechanism, which is triggered by dropping a weight down along the measuring tape to which the probe is attached.

Multiple laboratory and field tests are conducted to evaluate the injection probe. Especially the extent and reproducibility of the generated tracer profile are assessed by several experiments in an acrylic glass well. Repeated injections show an almost identical concentration curve, proving that the invented probe is able to reproduce the initial tracer cloud. Also, the opening mechanism proves to be robust and reliable. The probe can be operated by a single person and is suitable for any kind of soluble tracer. Moreover, it can be used in any aquifer type and is highly flexible regarding injection depths, which gives the probe several advantages compared to conventional methods

The third study summarizes the results of all conducted tracer-based experiments and evaluates the outcomes with regard to the groundwater protection area Donauried-Hürbe in order to obtain a multi-scale characterization of the aquifer system. Particular focus lies on the inflow towards the Danube valley and the extraction wells of the Zweckverband Landeswasserversorgung. While SBDTs are used to observe flow processes on a local scale, large-scale groundwater flow is investigated with a regional multi-tracer test that was started in October 2017 in cooperation with the regional water supplier (Zweckverband Landeswasserversorgung).

The investigations of selected groundwater monitoring wells prove a broad range of results, especially regarding outflow times. While wells with a good connection to the karst conduits and wells located in highly permeable areas of the alluvial aquifer document fast tracer outflow, long outflow times of up to several days are observed in wells in low-permeable formations. 40 % of the tested groundwater monitoring wells show vertical flow caused by the complex aquifer hydraulics. With the multi-tracer test, high groundwater flow velocities of around 80 m/h are observed between the swallow hole in the Lone valley and a karst spring group in Langenau. However, exceptionally delayed breakthroughs with first arrivals of 250 and 307 days after the injection are also documented, resulting in maximum flow velocities of only 0.44 and 0.39 m/h.

Until April 2023, no tracer was detectable in the extraction wells of the Zweckverband Landeswasserversorgung.

In summary, the results of the tracer methods used in this thesis attest the distinct cross-scale heterogeneity of the groundwater flow in the protection area Donauried-Hürbe. In addition to the methodological enhancements of the SBDTs, this thesis substantially contributes to a deeper understanding of the complex aquifer system with its importance for the water supply of three million people in southern Germany.

KURZFASSUNG

Grundwasser ist die wichtigste Ressource für die Trinkwasserversorgung in Deutschland sowie in zahlreichen Ländern weltweit. Dürren, Starkregen und steigende Evapotranspiration, Phänomene die durch den Klimawandel verstärkt werden, reduzieren die verfügbare Menge an Grundwasser. In Kombination mit einem steigenden Bedarf aufgrund höherer Temperaturen, ist die Aufrechterhaltung einer funktionierenden und nachhaltigen Wasserversorgung eine der wichtigsten und dringendsten Aufgaben denen sich Wasserversorger aktuell stellen müssen. Zur Entwicklung und Umsetzung notwendiger Anpassungsmaßnahmen sind gute Kenntnisse der Grundwasserressourcen notwendig, welche lediglich durch detaillierte Untersuchungen der Einzugsgebiete und Grundwasserleiter erreicht werden können.

In dieser Thesis wird das komplexe System eines Karstaquifers in Kombination mit einem alluvialen Grundwasserleiter im Grundwasserschutzgebiet Donauried-Hürbe untersucht. Es umfasst einen großen Teil der östlichen Schwäbischen Alb sowie des baden-württembergischen Donautals und wurde für die über 200 Entnahmebrunnen im Donauried ausgewiesen, die durch den Zweckverband Landeswasserversorgung betrieben werden. Das dort entnommene Wasser trägt zur Trinkwasserversorgung von ca. 3 Millionen Menschen in Süddeutschland bei, inklusive der Metropolregion Stuttgart. Ziel dieser Thesis ist eine skalenübergreifende Charakterisierung des Einzugsgebiets der Entnahmebrunnen, insbesondere im Hinblick auf den Zustrom zum Donautal. Während Einzel-Bohrloch-Verdünnungsversuche (single-borehole dilution tests, SBDTs) für die kleinskaligen Untersuchungen eingesetzt werden, erfolgt die großmaßstäbliche Betrachtung mittels eines kombinierten Markierungsversuchs.

SBDTs sind eine Markierungsmethode zur Charakterisierung von Grundwassermessstellen sowie Bohrlöchern. Sie können in allen Aquifertypen angewendet werden – besonders interessant sind heterogene Karst- und Kluftaquifere – und können mittels uniformer Eingabe oder Punkteingabe durchgeführt werden. Uniforme Eingaben streben eine homogene Konzentration des Markierungsmittels über die gesamte gesättigte Länge eines Bohrlochs an und liefern Informationen über maßgebliche Zu- und Abflusshorizonte. Wenn keine vertikalen Strömungen auftreten, können zudem horizontale Filtergeschwindigkeiten berechnet werden. Bei der geläufigsten Methode für uniforme Eingaben wird ein Schlauch zur Injektion gelöster Markierungsstoffe eingesetzt.

In der ersten Studie wird eine vereinfachte Methode für uniforme Eingaben unter natürlichen Fließbedingungen entwickelt, geprüft und mit der gängigen Schlauchmethode verglichen. Die neue Methode nutzt einen permeablen Injektionsbeutel (PIB), um eine möglichst gleichmäßige Verteilung des Markierungsstoffs in der gesättigten Zone zu erreichen. Die PIB-Methode wird für eine Vielzahl an Tests im Labor und in mehreren Grundwassermessstellen im

Untersuchungsgebiet eingesetzt, um eine fundierte Beurteilung zu ermöglichen. Wiederholte Tests in ausgewählten Messstellen werden durchgeführt, um die Reproduzierbarkeit der Methode zu untersuchen. Darüber hinaus werden zwei unterschiedliche Berechnungsmethoden basierend auf linearer Regression sowie der eindimensionalen Advektions-Dispersions-Gleichung genutzt, um scheinbare horizontale Filtergeschwindigkeiten zu berechnen. Die Ergebnisse belegen, dass die PIB-Methode für die untersuchten Grundwassermessstellen wertvolle und reproduzierbare Daten generiert. Außerdem ist sie äußerst flexibel im Hinblick auf die Tiefe der Messstellen, benötigt weniger Ausrüstung als vergleichbare Methoden und kann von einer einzelnen Person durchgeführt werden.

In der zweiten Studie wird eine Sonde für SBDTs mit Punktinjektion vorgestellt, die im Rahmen dieser Thesis entwickelt und getestet wird. Mit der Injektion eines Markierungsmittels in einem spezifischen Tiefenbereich wird eine detaillierte Untersuchung der Fließprozesse in dieser Tiefe ermöglicht. Darüber hinaus produzieren uniforme Injektionen oftmals keine eindeutigen Ergebnisse hinsichtlich vertikaler Fließbewegungen, welche besonders in Karst- oder Kluftaquiferen häufig auftreten; Punktinjektionen hingegen sind explizit zur Untersuchung von Vertikalbewegungen geeignet. Die Kenntnis vertikaler Grundwasserströmungen ist essentiell für das Verständnis hydraulischer Prozesse in komplexen Aquifersystemen. Die entwickelte Injektionssonde ist darauf ausgelegt, 500 mL Markierungsstofflösung in einer beliebigen Tiefe freizusetzen, ohne den natürlichen Grundwasserfluss durch den Injektionsprozess zu verändern. Die Sonde besteht aus einem hohlen Zylinder mit einem Öffnungsmechanismus, der durch ein Fallgewicht entlang des Maßbandes ausgelöst wird, an welchem die Sonde befestigt ist.

Zur Evaluierung der Injektionssonde werden zahlreiche Labor- und Feldtests durchgeführt. Besonders werden mittels mehrerer Versuche in einem Acrylglasrohr Ausdehnung und Reproduzierbarkeit des generierten Injektionsprofils untersucht. Wiederholte Eingaben zeigen jeweils eine nahezu identische Konzentrationskurve, wodurch bestätigt wird, dass die entwickelte Sonde eine reproduzierbare Tracerwolke erzeugt. Außerdem erweist sich der Öffnungsmechanismus als robust und verlässlich. Die Sonde kann von einer einzelnen Person und mit jeglichem lösbaren Markierungsmittel eingesetzt werden. Darüber hinaus ist sie für jeden Aquifertyp geeignet und äußerst flexibel bezüglich der Eingabetiefe, wodurch die Sonde im Vergleich mit gängigen Methoden zahlreiche Vorteile aufweist

Die dritte Studie fasst die Ergebnisse aller durchgeführten Markierungsversuche zusammen und wertet die Resultate bezogen auf das Grundwasserschutzgebiet Donauried-Hürbe aus, mit dem Ziel eine skalenübergreifende Charakterisierung des Aquifersystems zu erreichen. Besonderer Fokus wird dabei auf den Zustrom zum Donautal und den Entnahmebrunnen des Zweckverbands Landeswasserversorgung gelegt. Während mit den Ergebnissen von SBDTs kleinräumige Fließprozesse evaluiert werden, wird der regionale Grundwasserfluss mit einem kombinierten

Markierungsversuch untersucht, der im Oktober 2017 in Zusammenarbeit mit dem regionalen Wasserversorger (Zweckverband Landeswasserversorgung) gestartet wurde.

Die Untersuchungen ausgewählter Grundwassermessstellen belegen eine große Bandbreite an Ergebnissen, besonders im Hinblick auf die Abflusszeiten. Während Messstellen mit einer guten Anbindung an die Karströhren sowie Messstellen in hochdurchlässigen Bereichen des alluvialen Aquifers einen schnellen Abstrom des Markierungsmittels zeigen, werden in Messstellen geringdurchlässiger Formationen lange Abflusszeiten von bis zu mehreren Tagen festgestellt. 40 % der untersuchten Grundwassermessstellen zeigen vertikale Strömungen, die auf die komplexe Hydraulik des Aquifersystems zurückzuführen sind. Mit dem kombinierten Markierungsversuch werden hohe Fließgeschwindigkeiten von etwa 80 m/h zwischen der Schwinde im Lonetal und einer Quellgruppe in Langenau beobachtet. Jedoch werden ebenfalls äußerst verzögerte Durchgänge mit Ersteinsätzen von 250 und 370 Tagen nach der Eingabe dokumentiert, woraus maximale Fließgeschwindigkeiten von lediglich 0.44 und 0.39 m/h resultieren. In den Entnahmebrunnen des Zweckverbands Landeswasserversorgung ist bis einschließlich März 2023 kein Markierungsmittel nachweisbar.

Zusammenfassend belegen die Ergebnisse der eingesetzten Markierungsmethoden die ausgeprägte und skalenübergreifende Heterogenität des Grundwasserflusses im Schutzgebiet Donauried-Hürbe. Zusätzlich zu den methodischen Weiterentwicklungen von SBDTs, trägt diese Thesis wesentlich zu einem tieferen Verständnis des für die Wasserversorgung von drei Millionen Menschen in Süddeutschland essentiellen und komplexen Aquifersystems bei.

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CHAPTER 1

1 Introduction

1.1 General motivation

A well-functioning water supply is one of the most important bases for the development of a country or region. In addition to the provision of clean drinking water, it is also essential for food production and sanitation, but also for industrial development and the generation of jobs (Olmstead 2014; United Nations 2015; Stevanović 2019). Worldwide, groundwater is the most widely used resource for drinking water supply, as it is the safest and most reliable source of water (Aureli 2010). More than 50 % of mankind relies on groundwater resources for drinking water and at least 2.5 billion people are solely dependent on groundwater as water source (United Nations Educational, Scientific and Cultural Organization 2015; Konikow and Bredehoeft 2020). Due to climate change and an increasing demand – mainly due to population growth and an increasing standard of living – groundwater resources are under pressure in many parts of the world, including European countries (Green et al. 2011; Kløve et al. 2014; Wang et al. 2016; Stevanović 2019).

Still, not enough information about the effects of climate change on groundwater resources are available, especially due to the fact that climate change affects hydrological processes and groundwater resources directly, for example due to a higher evapotranspiration, and indirectly, for instance through a change of accumulated precipitation or an increasing demand due to higher temperatures (Kløve et al. 2014; Dettinger et al. 2015; Teuling et al. 2019; Deutscher Verein des Gas- und Wasserfaches e.V. 2022). Additionally, the properties of important aquifers are often not sufficiently known, as well as the impact of human activities (Green et al. 2007; Wang et al. 2016). Further research as well as a detailed investigations of relevant aquifer systems are necessary to develop adequate adaption strategies and to improve the resource management, in order to mitigate the effects of climate change and secure the future water supply.

In Germany, too, groundwater is the most important resource for water supply. In 2008, the German Federal Government published the German climate change adaption strategies (Bundesregierung 2008), predicting that no major effects would result from changes climate conditions. Only local exceptions caused by droughts were considered possible (Bundesregierung 2008). In the second monitoring report concerning the adaption strategies from 2019, however, a widespread trend towards an increasing number of historically low groundwater levels is confirmed (Umweltbundesamt 2019). Thus, further climate change-related impacts on groundwater resources will also occur in Germany (Deutscher Verein des Gas- und Wasserfaches e.V. 2022).

German federal states are also monitoring the effects of climate change on water supply, proving that the importance of this issue is now recognized in politics. In the state of Baden-Württemberg, a master plan for water supply ("Masterplan Wasserversorgung") was launched in 2020 (Ministerium für Umwelt, Klima und Energiewirtschaft Baden-Württemberg 2020). This master plan takes into account not only the development of groundwater resources, but also the water demand forecast until 2050. As a final result, recommendations are to be formulated for each municipality, in order to adapt and secure drinking water supply in the face of climate change. The first step, however, is the data acquisition of the current state of all water supply infrastructure and the detailed monitoring and investigation of water resources and aquifers (Ministerium für Umwelt, Klima und Energiewirtschaft Baden-Württemberg 2020).

The Zweckverband Landeswasserversorgung (state water supply, LW) in Baden-Württemberg, one of Germany's largest water suppliers, strives to increase the knowledge of the managed groundwater resources and to improve the already existing data base on groundwater flow and aquifer properties. Not only for the adaptions to climate change effects, but also to prepare for potential contaminations and increasing nitrate concentrations (Haakh 2018, 2019), the LW wants to further characterize the managed aquifer system and to gain data about groundwater hydraulics, flow paths and velocities. Investigating the catchment of the LW´s extraction wells is difficult due to a complex combination of a karst aquifer and an alluvial aquifer (Schloz et al. 2007). While the largest part of the required groundwater is extracted from the alluvial aquifer in the Danube Valley (Zweckverband Landeswasserversorgung 2012), the main recharge area is the low mountain range of the eastern Swabian Alb, built up by Jurassic limestones that form a large karst aquifer (Kolokotronis et al. 2002).

Karst aquifers have a special role among groundwater resources. Around 14 % of the ice-free land surface is karst, and more than 9 % of the world population obtain their water from karst aquifers (Stevanović 2019). Karst aquifers are especially vulnerable to pollution, overexploitation and climate change effects, which is why they require special management and protection strategies, in order to maintain a good water quality and to sustain the resource (Bakalowicz 2005; Ford and Williams 2007; Goldscheider and Drew 2007; Stevanović 2019).

Karst aquifers are particularly challenging as, unlike than sand or gravel aquifers, they show a dual porosity caused by karstification processes, which corresponds to the pores of the rock matrix and enlarged conduits or fractures. This duality leads to a complex flow behaviour and a distinct heterogeneity that complicates managing or investigating these aquifers (Bakalowicz 2005; Goldscheider and Drew 2007).

The combination of rock matrix and conduits also leads to varying flow behavior during different hydraulic conditions. In times of high flow, water infiltrates from the conduits into the rock matrix, whereas low-flow conditions lead to an inverted flow regime and a drainage of the matrix pores through the conduits (Martin and Dean 2001; Frank et al. 2019). This phenomenon also applies to the transport of soluble substances, for example in case of a contamination. High pollutant concentrations in the conduits lead to an infiltration into the rock matrix. After the concentration in the conduits falls below the concentration in the matrix, the gradient is inverted, leading to a diffusion-controlled transport back into the conduits. This results in lower maximum concentrations at springs or extraction wells, but consequently to a long ongoing contamination (Li et al. 2008; Ghasemizadeh et al. 2012; Xu et al. 2015).

Another challenge that karst aquifers naturally bring with them and that complicates their examination is the conductivity scale effect. This effect corresponds to the difference in observable hydraulic conductivities with regard to the investigated scale (Kiraly 1975; Jazayeri Noushabadi et al. 2011; Hartmann et al. 2014; Medici and West 2021). On the laboratory scale, most experiments with drilling cores only deliver information about the rock matrix, which usually shows low conductivities (***Figure 1***). The investigation of boreholes, the next larger scale, can document matrix dominated flow as well as conduit dominated flow, which leads to a wider range of results and typically higher hydraulic conductivities compared to drilling cores. Regarding entire karst aquifers, the influence of conduits exceeds matrix influences (Jazayeri Noushabadi et al. 2011). Especially strongly karstified aquifers in combination with high-flow conditions lead to almost exclusively conduit-dominated flow and thus high conductivities. However, in an early stage of karstification, karst aquifers can still show low, matrix-dominated hydraulic conductivities, especially during low-flow conditions (Hartmann et al. 2014). The scale effect applies not only to the hydraulic conductivities, but also to hydraulic transport parameters like dispersivity, diffusion or sorption as well as reaction rates, which further complicates the understanding of aquifer processes, especially in karst aquifers (Zhang et al. 2021).

Due to the general heterogeneity as well as the conductivity scale effect, karst aquifers are difficult to investigate and demand special investigation methods (Goldscheider and Drew 2007; Armbruster et al. 2008). Often a combination of different methods is required; for instance, different tracing techniques can be used to assess different properties or scales of a karst aquifer (Goldscheider and Drew 2007; Armbruster et al. 2008). Since different hydraulic conditions can lead to varying results, a repetition of tests is necessary to cover the wide range of possible flow properties that occur in karst aquifers.

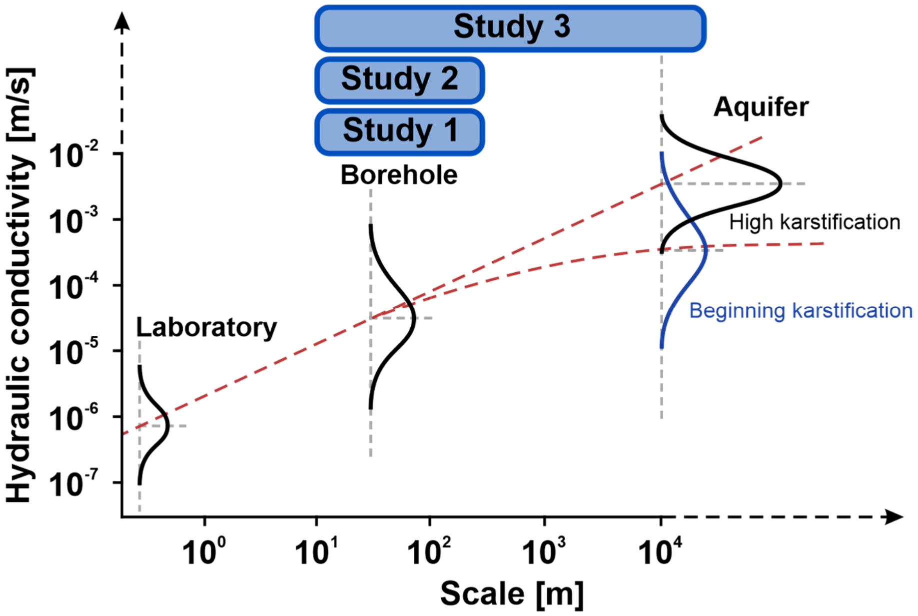

Figure 1: *Hydraulic conductivity-scale effect in karst aquifers modified after Kiraly (1975) and Hartmann et al. (2014). The larger the scale, the more the influence of karstification increases, resulting in higher hydraulic conductivities. With study 1 (**Chapter 2**) and study 2 (**Chapter 3**) hydraulic conductivities are investigated on the borehole scale, study 3 (**Chapter 4**) also includes the aquifer scale.*

1.2 Methods for aquifer investigation

Most aquifer investigation methods are non-specific with respect to the hydrogeological setting and can in principle be applied in all aquifer types (Goldscheider and Drew 2007). However, the significance of the results and especially the scale of the representative area may vary depending on the hydrogeological setting. One method that is almost solely limited to karst areas are **speleological investigations** as they study caves and cavities. Especially in large cave systems, for example the Blauhöhle in Germany, valuable insights in flow behavior and history of an aquifer history can be obtained (Abel et al. 2002; Goldscheider and Drew 2007; Goldscheider 2008; Strasser et al. 2009; Lauber et al. 2013).

In many cases and especially in smaller catchments, **spring monitoring** is sufficient to identify relevant flow characteristics of an aquifer. For example, dissolution and dilution processes as well as response times to precipitation events can be investigated based on water chemistry. Also, mobilisation and transport of contaminants like fecal bacteria can be explored with the help of spring monitoring (Mudarra et al. 2014a; Frank et al. 2019, 2022; Jutglar et al. 2021; Vucinic et al. 2022).

One other group of investigation methods are **tracing techniques**, which were initially developed and utilized in karst areas, but are nowadays applied in all aquifer types, mainly in order to identify flow paths and velocities (Käss 1992). Also, tracer tests deliver necessary input data for the setup of numerical models. Tracing techniques can be divided in artificial and natural tracer methods and are applicable on different scales. Natural tracer methods refer to the evaluation of water chemistry or natural suspended particles, but also to accidental inputs, for example due to a leakage. Artificial tracers, on the other hand, are injected as part of a planned test. Mostly fluorescence dyes, salts and various particle tracers are used (Käss 1992; Goldscheider 2008).

Aside from field tests, tracer methods are also used for small-scale laboratory tests, for example column or tank experiments to investigate transport parameters or interactions between different tracers and rocks or sediments (Käss 1992; Eriksson et al. 1997; Guo et al. 2022; Huang et al. 2022). Regarding large-scale investigations, the chemical stability and the low detection limits of fluorescence dyes allow for tracer tests that cover long distances of several kilometers as well as long flow times of several months or even years (Gabrovšek et al. 2010; Lu et al. 2011; Petrič et al. 2018).

Borehole methods offer a possibility to investigate specific points within an aquifer. The most common borehole investigations are pumping tests to determine hydraulic aquifer parameters. Based on the extraction rates and the drawdown of the water level, transmissivity, permeability and specific storage can be calculated (Hölting and Coldewey 2013). Pumping tests can also be conducted in combination with borehole packers, in order to obtain flow parameters for different depth intervals (Le Borgne et al. 2007; Quinn et al. 2012).

Other common borehole methods are geophysical investigations of the hydraulic or stratigraphic properties, for example with the use of caliper logs, gamma-ray logs as well as measurements of temperature or electrical conductivity profiles (Hölting and Coldewey 2013). One way to identify and to quantify borehole flow properties are flowmeter measurements. With an impeller meter, vertical flow within a borehole is measured in undisturbed conditions as well as while pumping with a constant extraction rate. Based on the measured flow rates while pumping, in- and outflow horizons can be identified and quantified as a percentage of the pumping rate (Molz et al. 1989; Paillet 2000; Le Borgne et al. 2006). Other borehole methods, for example the PHREALOG and PHREASIM combination that is based on the observation of moving suspended particles, are able to quantify flow velocities as well as outflow directions within a borehole (Drießen et al. 2015).

Independent of the aquifer type, the applicability of pumping tests or other borehole methods is limited due to varying aquifer thickness or heterogeneous sedimentation, but especially in heterogeneous karst aquifers. Obtained results are only representative for a small scale, namely the area that was covered with the respective test (Goldscheider and Drew 2007; Hölting and Coldewey 2013). Also, to characterize an entire karst aquifer, a multitude of tests is necessary, resulting in a great effort and high expenses.

With multiple piezometers in one aquifer, already many questions regarding aquifer hydraulics can be answered based on the development of water levels (Villinger 1977). Additionally, effective porosity and also the water volume can be estimated (Bonacci 1995). However, due to the complexity, special care must be taken when interpreting the hydraulics of karst aquifers (Goldscheider and Drew 2007).

With the use of **numerical models**, groundwater flow and solute transport can be illustrated or prognosed. However, to set up a numerical model, the results of previous investigations, for example tracer tests or discharge data, are required as input parameters (Worthington 2009; Hartmann et al. 2014). In mostly homogeneous aquifers the results of a few pumping tests are sufficient to obtain the data to build an aquifer model. However, due to the heterogeneity as well as the combination of the often-complex conduit system and the rock matrix, karst aquifers are difficult to display with a numerical model (Scanlon et al. 2003; Worthington 2009; Chen and Goldscheider 2014).

Regarding the groundwater protection area Donauried-Hürbe, not all investigation methods are suitable. Spring monitoring does not provide enough insight on relevant processes and aquifer parameters, mainly due to the low number of springs and the large extent of the catchment area. Also, due to the complex geology and the karstification (***Chapter 1.3***, C***hapter 4.2.1***), numerical models are not able to display groundwater flow in the catchment correctly. However, a large number of groundwater monitoring wells were built in the study area (***Chapter 2.2.1***) that can be used for small-scale investigations, but also to generate important hydraulic data spatially distributed throughout the aquifer system.

For the characterization of the groundwater protection area Donauried-Hürbe two tracer-based methods are chosen: an artificial multi-tracer test for investigating the large-scale and single-borehole dilution tests (SBDTs) for detailed examinations. The advantage of a tracer test with a combined injection of different dyes at different injection sites is that multiple flow paths can be investigated simultaneously (Käss 1992; Goldscheider and Drew 2007). SBDTs, on the other hand, are suitable for examining the existing groundwater monitoring wells due to low costs and manageable effort.

SBDTs can be used to investigate groundwater flow in monitoring wells or boreholes and to identify the major flow horizons. They can be conducted using different kinds of tracers as well as various injection methods. After a tracer injection into the saturated zone, multiple concentration profiles are measured until the values return to the natural background (Freeze and Cherry 1979; Hall 1993; Maurice et al. 2011). In ***Table 2*** (***Chapter 2.1***), different SBDT-methodologies are listed, the methods used in this thesis are described in detail in ***Chapter 2.2.2*** and C***hapter 3.2***.

SBDTs can deliver results that are comparable to other borehole investigation methods. Like flow meter measurements, SBDTs are able to identify the major in- or outflow horizons, however, they cannot quantify the water flow. Regarding natural vertical flow, flow meter measurements can only detect natural vertical flow at high velocities, while dilution tests are able to identify minor vertical movement. General advantages of SBDTs are cost-efficiency and simplicity (Pitrak et al. 2007; West and Odling 2007; Maurice et al. 2011), which makes them also suitable for areas with many monitoring wells and, accordingly, a large number of required tests.

1.3 Groundwater protection area Donauried-Hürbe

Geography and cultural significance

The groundwater protection area Donauried-Hürbe is located in southern Germany at the border between the states of Baden-Württemberg and Bavaria (***Figure 2 a***). It extends over a large part of the eastern Swabian Alb, a low mountain range, and the Donauried, a segment of the Danube valley. With more than 500 km², Donauried-Hürbe is the largest groundwater protection area in Baden-Württemberg and one of the largest in Germany (Bundesministerium für Umwelt, Naturschutz und nukleare Sicherheit and Umweltbundesamt 2018). The dominant forms of land use are agriculture and forestry; however, several industrial parks and quarries are present within the protection area (Reumann 2006; Müller et al. 2019).

The Swabian Alb also has a high cultural value that, amongst other factors, was also favored by the large number of karst caves in the area (Krönneck et al. 2004). With more than 2800 documented caves, the Swabian Alb is the cave-richest region in Germany (Meister et al. 2021; Megerle 2022), many of which were used to live in early on. Already 35,000 – 40,000 years ago, the eastern Swabian Alb was populated as documented by the find of the oldest known musical instrument worldwide, a flute made from the bones of a griffon vulture (Münzel et al. 2002; Conard et al. 2009; Meister et al. 2021). The most famous discovery was made in the Lone valley: The Löwenmensch, a 31 cm tall sculpture of a man with a lion's head and limbs made out of mammoth ivory (Meister et al. 2021). Due to the cultural importance, the karst caves of the Swabian Alb were added to the list of UNESCO World Heritages in 2017 (United Nations Educational, Scientific and Cultural Organization 2017; Meister et al. 2021), which already includes a large number of karst areas, due to their rich biodiversity above and below surface as well as their landscape and historical value (Hamilton-Smith 2007; Goldscheider 2019).

In 2009, an area of 850 km² west of the groundwater protection area was designated as UNESCO Biosphere Reserve, especially due to the unique cultivated landscape and the initiatives for a sustainable interaction of man and nature (Bieling 2014; Meister et al. 2021). Additionally, almost the entire Swabian Alb was designated as national Geopark in 2002, mainly due to the karst phenomena, fossil-richness and the extinct volcanism. In 2004 it was named European Geopark, and in 2015 the area with a total size of around 6,200 km² also became an UNESCO Global Geopark (Megerle 2020, 2021, 2022; Meister et al. 2021).

Geology

The groundwater protection area Donauried-Hürbe is dominated by Jurassic limestones that build up the low mountain range of the Swabian Alb and gently dip towards the southeast (Schloz et al. 2007). Originally, the limestones showed thicknesses of up to 600 m (Udluft et al. 2000; Schmid et al. 2005; Meister et al. 2021); nowadays, due to intensive karstification since the Cretaceous, maximum thicknesses of around 400 m are existent (Schloz et al. 2007). Bedded facies as well as reef limestones occur, both of which can be fossil-rich (Gwinner 1976; Hegele 2010).

The low-permeable Lacunosa marls underneath the limestones represent the base of karstification in the study site, and hence are the deepest geological formation relevant for the investigated aquifer system (Schloz et al. 2007). A detailed description of the different formations of the Upper Jurassic can be found in Schmid et al. (2005).

The cliff line of the former Molasse Sea (“Klifflinie“) with a height difference of up to 50 m crosses the Swabian Alb from southwest to northeast (Kolokotronis et al. 2002). South of this line, deposits of Oligocene and Miocene Molasse occur with increasing extents and thicknesses towards the southeast (Geyer and Gwinner 1997). In the Danube valley, a widespread Molasse cover of the limestones with thicknesses of up to 90 m is given (Schloz et al. 2007).

On top of the Molasse, Quaternary gravels and sands were deposited that are covered by clay and silt and peat, resulting in thicknesses of up to 15 m (Schloz et al. 2007). Only at the border to the Swabian Alb, Molasse sediments were eroded by the Danube, resulting in Quaternary deposits lying directly on top of the limestones (Schloz et al. 2007).

Additionally, the geology of the groundwater protection area Donauried-Hürbe is described in C***hapter 4.2.1*** and a geological map is shown in ***Figure 20***.

Hydrogeology

The Jurassic limestones build up a large karst aquifer, which is recharged by precipitation in the area of the Swabian Alb infiltrating diffusely through swallow holes, epikarst and widespread shallow soils (Kolokotronis et al. 2002). Due to the latter, only a minor protection against pollutant infiltration into the karst aquifer is given (Wirsing and Kern 2020).

In the Danube valley, the Quaternary sediments form an alluvial aquifer, which is widely separated from the karst aquifer by the low-permeable Tertiary Molasse. However, trough faults, areas with low Molasse thicknesses and the area where the Molasse sediments were eroded by the Danube, karst groundwater can infiltrate into the alluvial aquifer (Schloz et al. 2007). A hydrogeological cross-section is displayed in ***Figure 21 (Chapter 4.2.1***).

For the Jurassic karst aquifer, the mean residence time was determined between 10 to 20 years using isotopes. However, 10 to 30 % of the groundwater is assumed to have a mean residence time of more than 50 years. Especially, wells close to the Danube that are poorly connected to upwelling karst groundwater show a higher percentage of old groundwater. On the other hand, springs with a direct connection to the karst conduits also show a fast flow component of up to 10 % of the total discharge with residence times of just a few days (Armbruster et al. 2008).

The European watershed crosses the groundwater protection area in the northwestern part, although the exact course of the watershed depends on the hydrological situation and the water level in the karst aquifer (Kolokotronis et al. 2002). Due to the special geological setting, only few springs are existent in the groundwater protection area Donauried-Hürbe. Except for the Lone spring in the western part of the study area, large karst springs can only be found in the town of Langenau. The hydrogeology of the study site is further described in ***Chapter 4.2.1***.

1.4 Zweckverband Landeswasserversorgung (state water supply)

The groundwater protection area Donauried-Hürbe was established for the extraction wells of the Zweckverband Landeswasserversorgung (state water supply, LW), which is one of the largest long-distance water suppliers in Germany. The LW was founded as early as 1912 to secure the previously critical water supply of Stuttgart and the eastern Swabian Alb (***Chapter 4.1***). Nowadays, the LW provides high-quality drinking water for 106 association members with around three million inhabitants, including parts of the Stuttgart metropolitan region, which has a significant economic importance for Germany and especially the automotive industry (Zweckverband Landeswasserversorgung 2012, 2023).

The required water is extracted from the Danube, a large karst spring in Dischingen, five deep karst wells and 204 wells in the alluvial aquifer the Danube valley. Due to its good quality, groundwater from the alluvial aquifer in the Danube valley used to be the main water source for the LW (***Table 1***). As to allow for a recharge of the groundwater resources, which are essential for high-demand periods during summer, the usage of Danube water has been increased in the last years. However, even during low-flow conditions, still less than 1 % of the Danube's total discharge is extracted (Zweckverband Landeswasserversorgung 2012, 2023).

After treatment, the water is delivered to the association members through a large pipeline network with a total length of almost 775 km and a maximum delivery rate of 5,200 L/s (***Figure 2 b***). While the 33 water reservoirs managed by the LW have a total capacity of 400,000 m³, the pipeline network itself has a volume of around 350,000 m³. Several turbines with a total capacity of 6.4 MW are included in the pipeline network and generate green electricity that is reused in the water works (Zweckverband Landeswasserversorgung 2023).

Table 1: *Overview of recent extraction and delivery numbers of the LW. Groundwater total includes the water from the Danube valley (204 alluvial wells, 2 artesian karst wells) and three wells in Burgberg, which extract additional karst groundwater in times of high demand (Zweckverband Landeswasserversorgung 2012, 2016, 2020, 2021).*

	2010	2015	2018	2019	2020
Danube valley [Mio. m³]	35.7	30.2	29.6	23.9	28.9
Groundwater total [Mio. m³]	39.9	39.6	35.8	33.4	37.7
Buchbrunnen spring [Mio. m³]	17.6	14.8	15.0	17.0	15.7
Danube [Mio. m³]	30.2	37.1	48.9	54.6	45.5
Mean extraction value [m³/d]	248,717	259,979	283,155	270,530	277,719
Max. extraction value [m³/d]	353,345	409,334	369,579	362,529	374,574
Total water delivery [Mio. m³/a]	87.9	93.8	102.7	98.3	101.7

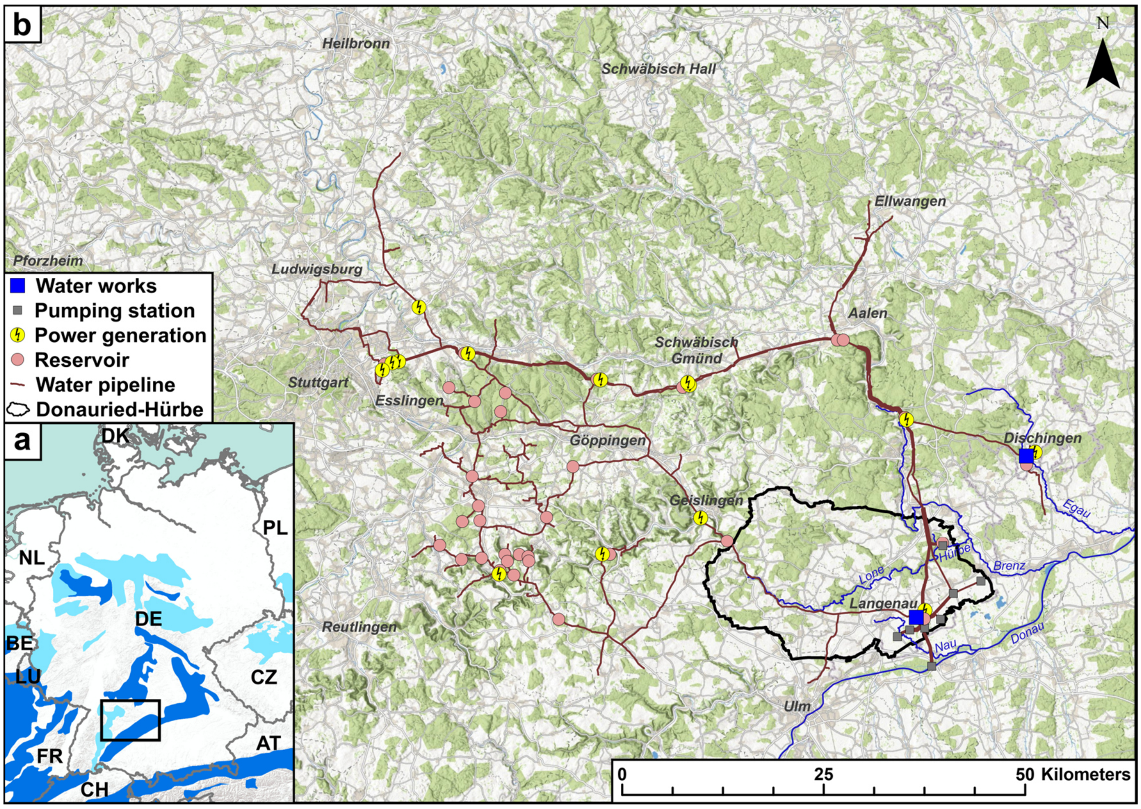

Figure 2: ***(a)*** *Location of the detailed map (black square) shown on a cut-out of the World Karst Aquifer Map (WOKAM, Chen et al. 2017); dark blue: continuous carbonate rocks, light blue: discontinuous carbonate rocks; country codes from International Organization for Standardization 2023).* ***(b)*** *Map of the region supplied by the LW including the pipeline network with a total length of 775 km and diameters between 0.7 and 1.5 m (Zweckverband Landeswasserversorgung 2023).*

Current challenges the LW has to face are declining groundwater levels and extreme weather events, both caused by climate change. In preparation of a predicted further intensification of these effects as well as to secure water supply in the future, the LW is evaluating new options to develop further resources (Haakh 2019; Zweckverband Landeswasserversorgung 2021).

With regard to water quality, especially high nitrate concentrations are problematic. A mass balance study (Haakh 2018) revealed that 86.5 % of the nitrogen compounds found in the water can be attributed to the intense agriculture in the groundwater protection area and in particular to the application of manure and digestate that exceeds regulations. In order to reduce nitrate concentrations, the LW advocates the consistent implementation of official fertilizer regulations (Haakh 2018).

1.5 Objectives and Approaches

The general objective of this thesis is to achieve a multi-scale characterization of a complex aquifer system with the use of different tracer methods at the example of the supra-regionally important catchment of the extraction wells in the groundwater protection area Donauried-Hürbe. By the use of SBDTs, selected groundwater monitoring wells at the study site are tested in order to generate important hydraulic data at several points distributed throughout the groundwater protection area. For this purpose, the development of a simplified and cost-efficient method for uniform-injection SBDTs is the first objective of this thesis. Since the groundwater monitoring wells show a high variability regarding depth and saturated length, the new method must be universally applicable. Furthermore, vertical flow in the aquifer system should be investigated with point-injection SBDTs, in order to understand the hydraulics in the aquifer system. Due to the lack of a suitable point injection device on the market, the second methodological objective is to develop an injection probe for detailed investigations of groundwater monitoring wells and boreholes. These objectives result in the following methodological research questions that are addressed in this thesis:

1. Can a simplified method for uniform injection SBDTs be developed?
2. Does the simplified method deliver reproducible results?
3. Is the simplified method applicable in different aquifer types and wells or boreholes with varying depths?
4. Can a cost-efficient injection device for point injections in groundwater be designed?
5. Does the injection device generate reproducible tracer profiles?
6. Can the injection device be used to investigate groundwater monitoring wells and especially vertical flow?

In combination with a regional multi-tracer test, SBDTs are used to characterize the aquifer system in the groundwater protection area Donauried-Hürbe across different scales. Therefore, the following research questions arise with regard to the study site:

7. Can SBDTs be used to draw conclusions about groundwater flow in a large and complex aquifer system with only few springs but many groundwater monitoring wells?
8. Can point-injection SBDTs be used to identify areas of rising or sinking groundwater?

9. What are the residence times from points with an increased contamination risk to the springs in Langenau and the wells in the Danube valley?
10. What is the range of flow velocities in the groundwater protection area Donauried-Hürbe and can hydraulic connections as well as sub-catchments in the study site be identified based on the multi-tracer test?
11. Is it possible to achieve a hydrogeological characterization of a complex aquifer system by the use of tracer methods only?

1.6 Scope and Structure of the thesis

The presented thesis has a cumulative structure and contains three peer-reviewed studies on different tracing methods for aquifer characterization, one of which lead to a patenting process for a designed injection probe. ***Chapter 2*** presents a newly developed and simplified method for uniform-injection SBDTs under undisturbed natural flow conditions. It uses a permeable injection bag to distribute the tracer throughout the entire saturated length of a monitoring well or borehole. The new method was tested in both the alluvial and the karst aquifer, as well as in wells with high and low flow velocities and varying depths. Also, the reproducibility of the generated results was evaluated and a comparison with the most common hosepipe method was conducted.

Chapter 3 introduces a newly developed probe for point-injection SBDTs that releases a tracer solution in a specific depth. Since no common method or device for point injections in groundwater is currently existent, a reliable and cost-efficient probe was designed that can be used in various settings with regard to aquifer type, depth or tracer. Since the resulting point injection probe fulfills all requirements and the opening mechanism is reliable, a patenting process was started that is still ongoing.

Chapter 4 summarizes the results of 51 SBDTs and one large-scale multi-tracer test in the study area Donauried-Hürbe. Based on different tracer methods, a cross-scale characterization of the aquifer system was achieved. While the borehole investigations displayed small-scale results on groundwater flow, the multi-tracer test allowed conclusions about flow paths with lengths of several kilometers.

Chapter 5 recapitulates the gained insights of all studies, highlights the major finding and puts them in the context of the catchment's importance for the water supply of the metropolitan area Stuttgart. Furthermore, an outlook on potential applications and further improvements of the developed methods and the point injection probe is given, as well as on additional research in the study site.

Additional research within the scope of the international research project KARMA (Karst Aquifer Resources availability and quality in the Mediterranean Area, Grant Agreement number 01DH19022A) lead to a co-authored study (Frank et al. 2022) on water quality at two alpine karst springs, which is not included in this thesis. Based on a monitoring of the fecal indicator bacteria *E. coli*, particle load, chemistry as well as organic matter, parameters for early-warning systems were identified. To observe contamination with fecal bacterial in near real-time, a novel method measuring the activity of β-D-glucuronidase – an enzyme that almost exclusively occurs in *E. coli* bacteria – was used.

CHAPTER 2

2 Comparative application and optimization of different single-borehole dilution test techniques

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Abstract

Single-borehole dilution tests (SBDTs) are a method for characterizing groundwater monitoring wells and boreholes, and are based on the injection of a tracer into the saturated zone and the observation of concentration over depth and time. SBDTs are applicable in all aquifer types, but especially interesting in heterogeneous karst or fractured aquifers. Uniform injections aim at a homogeneous tracer concentration throughout the entire saturated length and provide information about inflow and outflow horizons. Also, in the absence of vertical flow, horizontal filtration velocities can be calculated.

The most common method for uniform injections uses a hosepipe to inject the tracer. This report introduces a simplified method that uses a permeable injection bag (PIB) to achieve a close-to-uniform tracer distribution within the saturated zone. To evaluate the new method and to identify advantages and disadvantages, several tests have been carried out, in the laboratory and in multiple groundwater monitoring wells in the field. Reproducibility of the PIB method was assessed through repeated tests, on the basis of the temporal development of salt amount and calculated apparent filtration velocities. Apparent filtration velocities were calculated using linear regression as well as by inverting the one-dimensional (1D) advection-dispersion equation using CXTFIT.

The results show that uniform injection SBDTs with the PIB method produce valuable and reproducible outcomes and contribute to the understanding of groundwater monitoring wells and the respective aquifer. Also, compared to the hosepipe method, the new injection method requires less equipment and less effort, and is especially useful for deep boreholes.

2.1 Introduction

Investigation of boreholes with single-well methods plays an important role in hydrogeological aquifer characterization, especially in large and deep aquifers. Single-borehole dilution tests (SBDTs) are an easy-to-apply method for characterizing monitoring wells and boreholes and are based on the injection of a tracer into a borehole and the observation of the decreasing tracer concentration over time and depth. As a result, different flow regimes, in- and outflow horizons, and vertical flow in a borehole can be identified (Halevy et al. 1967; Freeze and Cherry 1979).

When vertical flow components are negligible or absent, SBDTs can also be used to determinate horizontal filtration velocities and their variation over depth (Hall 1993; Lamontagne et al. 2002; Bernstein et al. 2007; Maurice et al. 2011). Unlike other methods, for example flowmeter logging, SBDTs can also identify very low velocities (West and Odling 2007); however, obtained filtration velocities are just valid for a small area around the groundwater monitoring well (GMW) or borehole, but, for example, can still be used to predict the spreading rate of a pollutant at a specific location.

If GMWs or boreholes are to be used as injection points for classical tracer tests, for example where natural swallow holes are absent, a dilution test should be carried out before the injection, in order to examine the degree of hydraulic connection to the aquifer (Fahrmeier 2016). Especially in heterogenic karst aquifers, it is important to check if a GMW or borehole is connected to the active drainage network or not (Goldscheider and Drew 2007). If GMWs or boreholes are used as sampling points for tracer tests, SBDTs should be carried out to detect inflow horizons in order to choose the best sampling depths (Fahrmeier 2016). Results of SBDTs can also be used to determine sampling depths in monitoring wells and can also deliver additional information for the interpretation of other data, for example hydrochemistry (Poulsen et al. 2019a). Information gained from SBDTs can be complemented by drilling logs, since there is often a relation between lithology and outflow. With image logs in uncased boreholes, it is possible to observe the size and nature of the fissures or conduits contributing to the flow (Maurice et al. 2012). Geophysical methods can also contribute to a better understanding of flow horizons (Williams et al. 2006). If SBDTs are carried out under pumped conditions, transmissivities and storativities can be assigned to individual layers or fractures (West and Odling 2007).

SBDTs have several other potential applications whereby on the basis of their degree of connection to the aquifer and reaction times, the suitability of GMWs as observation points, e.g. near a quarry or a waste disposal site, can be checked. Additionally, SBDTs in multiple GMWs or boreholes in one aquifer could be used to obtain the range of occurring velocities and so contribute to the understanding of the system. Furthermore, the effectiveness of well-cleaning can be checked by performing a test before and after the cleaning process.

Two complementary types of injection can be used for SBDTs. Uniform injections aim at an even tracer concentration throughout the whole saturated length to get information about groundwater flow within the entire GMW or borehole and identify major flowing features. However, it is difficult to conclusively identify vertical flows from uniform injection data. For this and also for a detailed investigation of a particular depth, point injections need to be used (Maurice et al. 2011). Both uniform and point injections can be conducted using different techniques and injection devices, for example hosepipes or funnels, as well as different tracers, and with or without the use of pumps in the injection well or a GMW nearby (Palmer 1993; Shafer et al. 2010; Maurice et al. 2011). Packers can be used to separate defined segments of a borehole for detailed investigation, which, however, may cut off vertical flow (Drost et al. 1968; Grisak et al. 1977; Lamontagne et al. 2002). Point injections can also be conducted as continuous injections, typically by means of pumping, which also allows a quantification of flow rates (Poulsen et al. 2019b). ***Table 2*** provides an overview of examples from the literature with regard to tracer, methodology, and measuring devices. Early tests preferably used radioisotopes as tracers, because they allowed the determination of flow direction, using a scintillation counter (Drost et al. 1968; Klotz et al. 1979). Now mainly salts and fluorescence tracers (Halevy et al. 1967; Palmer 1993; Cook et al. 2001), as well as heated water (Leaf et al. 2012; Banks et al. 2014; Bense et al. 2016) or natural tracers, for example background conductivity (Love et al. 1999, 2003), are commonly used.

However, most of the existing methods still need a lot of equipment like packers or pumps, and at least two people. For these reasons, a method with reduced effort, easier handling, and less costs is needed. This report introduces a simplified uniform injection method for SBDTs under natural gradients and compares it to the hosepipe injection method. In order to compare the different methods and to identify their advantages and drawbacks, several SBDTs were conducted under laboratory conditions by the use of a Plexiglas tube and in GMWs in the field. Since SBDTs are preferably conducted in uncased boreholes to gain undisturbed results (Maurice et al. 2011; Jamin et al. 2015), also the applicability in GMWs with slotted casing was tested.

Table 2: *Summary of selected dilution tests from literature in chronological order.*

Author(s)	Tracer(s)	Injection	Methodology	Measuring method
Drost et al. 1968	Radioisotopes (NH482Br, 198Au, Na131I)	Point	Apparatus with two packers, mixing spiral, and injection syringe	Collimated scintillation-counter
Grisak et al. 1977	NaF	Point	Borehole dilution apparatus with two packers and mixing pump, tracer injection with peristaltic pump	Ion-selective electrode
Hall 1993	LiBr	Uniform	Hosepipe lowered into the borehole, filled with tracer solution, and then pulled out	12 ion-selective electrodes in different depths
Riemann et al. 2002	NaCl	Point	Circulating tracer with a pump in 2 m section, withdrawal 5 h after injection	Electrical conductivity sensor
Lamontagne et al. 2002	KCl, KBr	Point	Recirculation of the water in a sealed 0.5 m section with a peristaltic pump, injection with an in-line tracer reservoir	In-line electrical conductivity cell
Williams et al. 2006	NaCl	Uniform	Hosepipe lowered into the borehole, filled with salt solution and then removed	Electrical conductivity sensor
Bernstein et al. 2007	2,6-Difluorobenzoic acid	Point	Injection with peristaltic pump, mixing in injection well, forced gradient by pumping in a well 3 m away	Not specified by author
West and Odling 2007	NaCl	Uniform	Hosepipe lowered into the borehole, filled with salt solution and then removed, conducted near a pumped well	Electrical conductivity meter
Pitrak et al. 2007	Brilliant Blue FCF, NaCl	Uniform, Point	Plastic hose with syringes for point injection	Photometric sensor
Brouyère et al. 2008	Iodide, Lithium, Bromide, Uranine, Sulforhodamine B	Uniform	Circulation in the well with immersed pump, tracer injection with peristaltic pump	Samples taken before reinjection

Author(s)	Tracer(s)	Injection	Methodology	Measuring method
Gouze et al. 2008	Low salinity water, Uranine	Point	Withdrawal (push-pull) tests in a segment between two packers	Electrical conductivity sensor, optical sensor
Shafer et al. 2010	NaCl	Uniform	NaCl-solution injected with funnel and circulated with pump for 30 minutes (extraction near the bottom, reinjection on top)	EC profiles with electrical conductivity sensor
Maurice et al. 2011	NaCl	Uniform, Point	Hosepipe lowered into the borehole, filled with salt solution and then removed; point injection container filled with salt and opened by a weight dropped down the line	Electrical conductivity sensor
Leaf et al. 2012	Heated water	Point	Water is extracted in the cased part of the well, heated and reinjected in one or more depths	Fiber optic distributed temperature sensing
Banks et al. 2014	Heated water, NaCl	Uniform	Heated water: Electrical heating cables increase the temperature throughout the saturated zone NaCl: Starting at the bottom, tracer solution is pumped into the well through a hosepipe which is pulled upwards at a constant rate	Fiber optic distributed temperature sensing, multi parameter probe
Libby and Robbins 2014	Rhodamine WT	Uniform	Tracer pumped through hosepipe, starting at the bottom, then the pipe is pulled out, extraction at the top to maintain the static well head, afterwards mixing tool with propeller blades, combined with slug test	Optical probe attached to multiparameter probe
Jamin et al. 2015	Uranine	Point	Circulation between double packer system, injection with an in-line tracer reservoir	Field fluorimeter
Read et al. 2015	Heated water	Point	Discrete volume of water heated with point heater, combined with different extraction rates near the top	Fiber optic distributed temperature sensing
Poulsen et al. 2019b	NaCl	Point	Continuous point injection near one end of the well combined with extraction at the other end	Multi parameter probe
Yang et al. 2019	KCl, Rhodamine WT	Point	Isolation of a section with two packers, injection and recirculation between the packers with pumps	Electrical conductivity sensor, field fluorimeter

Three typical and generalized examples of developments of tracer concentration over time and depth typical for uniform injections are shown in ***Figure 3***. ***Figure 3 a*** shows a higher outflow rate in the upper part and a lower outflow rate beneath that, which leads to a faster decrease of salt concentration in the upper section and a slower decrease in the lower part. This development could represent a change of lithology, for example loamy sand with low permeability in the lower part overlain by gravel with a higher flow rate. ***Figure 3 b*** shows two outflow zones, with the upper one having a slightly higher flow rate. This could correspond to a borehole in a fractured or karst aquifer which intercepts two preferential flow horizons with the same hydraulic head, while ***Figure 3 c*** shows an inflow at the top, then a downward movement followed by an outflow at the bottom. This example would be typical for a GMW or borehole in a karst aquifer that connects two different conduits with higher hydraulic head in the upper one, or a well in a recharge area with downward movement of groundwater.

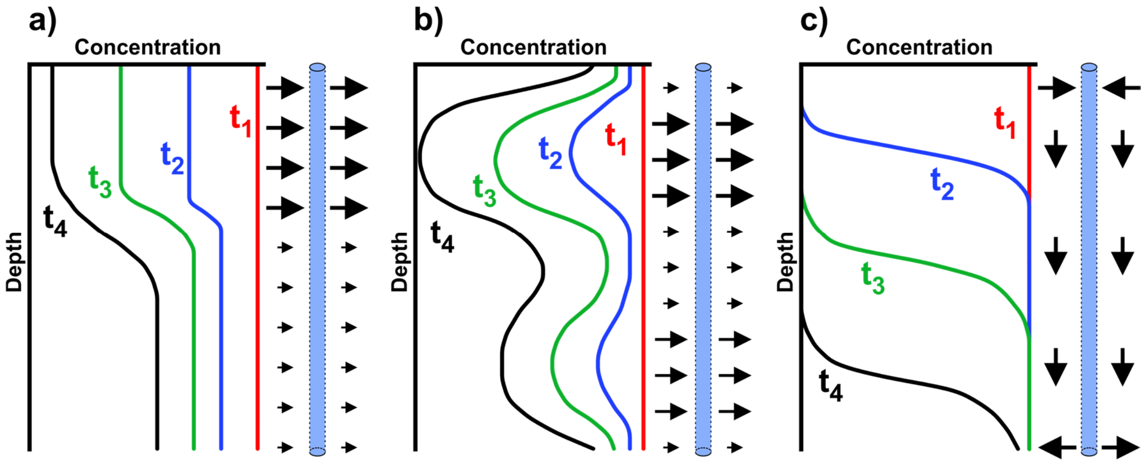

Figure 3: *Three typical patterns for the decrease of tracer concentration after uniform injections in monitoring wells (modified after Maurice et al. 2011). Curve t1 shows the ideal concentration after injection, while t2, t3 and t4 refer to increasing times after injection.* ***(a)*** *Shows higher flow in the upper part and lower flow in the lower part,* ***(b)*** *has two flow horizons one near the top, and one near the bottom;* ***(c)*** *shows vertical movement with inflow in the upper part and outflow near the bottom.*

2.2 Materials and methods

2.2.1 Study site

Field tests were performed in one of the largest groundwater protection areas in Germany *Donauried-Hürbe* (***Figure 4***), which was established for the extraction wells of the *Zweckverband Landeswasserversorgung* (state water supply) which provides high-quality drinking water for around 3 million people. It has a total area of over 500 km² and is located in the Federal State of Baden-Württemberg (Schloz et al. 2007).

The largest part of the study site, protection zone III, belongs to the eastern Swabian Alb, which is made up of Jurassic limestone with a thickness of up to 400 m that gently dips towards the southeast (Goldscheider 2005). In the south, the limestone is overlain by an increasing thickness of Tertiary Molasse sediments. In protection zone II, which corresponds to the Danube Valley, these sediments are up to 90 m thick. On top of the Tertiary formations, up to 10 m of Quaternary gravels and overlying silt and clay sediments of up to 7 m are present (Kolokotronis et al. 2002; Schloz et al. 2007). This geological setting leads to a complex hydrogeological system. The Jurassic limestones form a large and abundant karst aquifer, whose water flows to the southeast, where in some areas the Molasse is eroded, has just a small thickness, or is cut by fault zones. In those areas, water can flow from the karst into the gravel aquifer (Kolokotronis et al. 2002; Schloz et al. 2007).

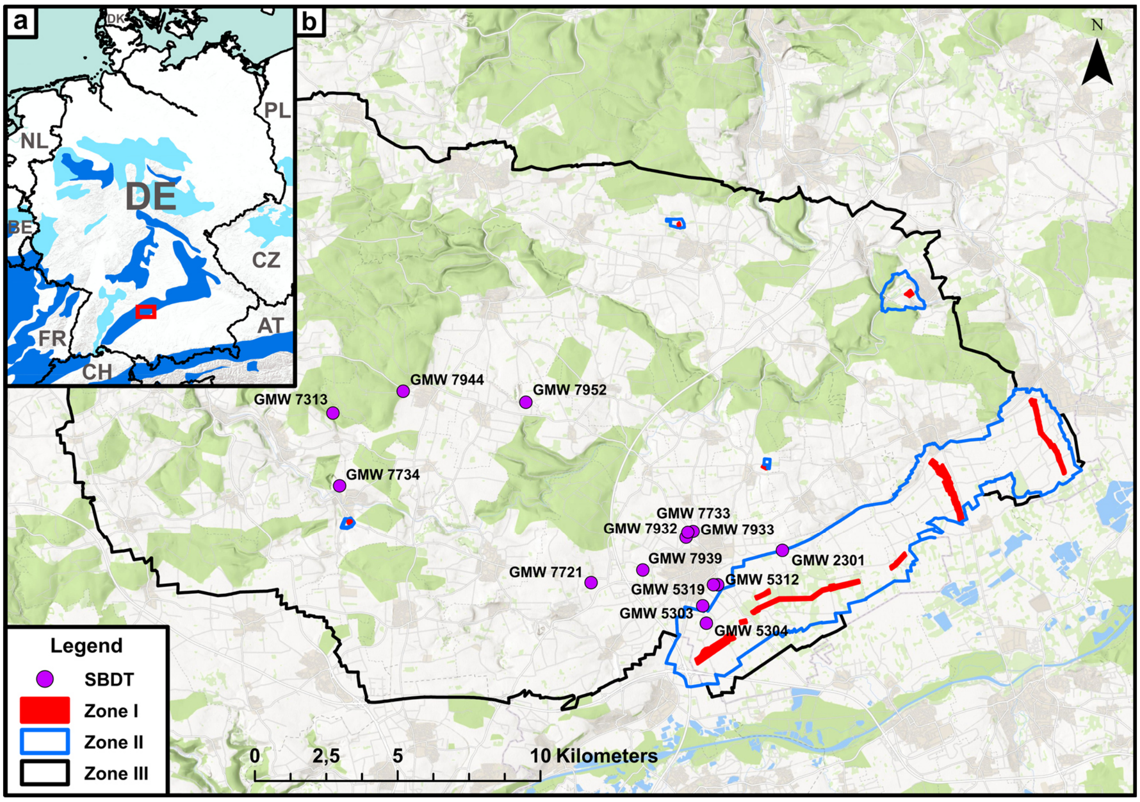

Figure 4: ***(a)*** *Location of the study site (red square) shown on a cut-out of the World Karst Aquifer Map (WOKAM, Chen et al. 2017; dark blue: continuous carbonate rocks, light blue: discontinuous carbonate rocks; country codes from International Organization for Standardization 2023).* ***(b)*** *Groundwater protection area "Donauried-Hürbe" with protection zones I, II and III (Schloz et al. 2007). Purple dots show GMWs in which SBDTs were conducted.*

More than 820 GMWs have been drilled in the study site since 1910 and equipped with slotted casing, 120 of them into the karst aquifer and 700 in the alluvial aquifer. Due to the large number of GMWs in two aquifers, SBTDs could be carried out under various conditions, with different depths to water level, saturated lengths, and outflow behaviors (***Table 3***). Within the scope of this work a total of 38 uniform injection SBDTs were conducted in 10 GMWs in the karst aquifer and in 4 GMWs in the gravel aquifer, using the permeable injection bag method and the hosepipe method. All SBDTs were conducted under undisturbed gradients and without the use of pumps. Additionally, four uniform injections were performed in a 6-m Plexiglas tube in the laboratory to test and compare the injection methods under fully controlled conditions, and to check for possible density effects during the experimental procedure.

2.2.2 Injection methods

2.2.2.1 Hosepipe method

Prior to every SBTD, the natural background of the used tracer within the GMW or borehole must be measured, and a calibration with the tracer and water from the respective GMW is required, to allow quantitative analyses. The most common method to obtain a uniform injection is the hosepipe method. A hosepipe is lowered into the GMW or borehole, with a weight attached at the end. Next, tracer solution is poured into the hosepipe, pushing the groundwater out of the lower end while replacing it with the tracer laden water (Maurice et al. 2011). The required amount of tracer solution can be calculated using the water level, well-depth and inner diameter of the used hosepipe. Injecting tracer in depth ranges with sealed casing can be avoided by pouring pure water into these sections of the hosepipe (West and Odling 2007). In conclusion, the hosepipe should be filled with tracer from the bottom to the water level or the upper end of slotted casing. The hosepipe is then pulled out, releasing the tracer into the surrounding water (***Figure 5 a***) To obtain a uniform injection, the hosepipe should be removed at a steady speed. The hosepipe method was used for six SBDTs during this study.

Due to low costs and easy measurability, saline solutions are predominantly used as tracer for SBDTs, also common is the usage of fluorescence dyes. Within the scope of this work, all tests were conducted using sodium chloride (NaCl) as tracer, due to easier handling compared to fluorescent dyes. Also, the outflow can be monitored easily by measuring depth profiles of electrical conductivity (EC); a TLC Meter Model 107 (Solinst Ltd.) and a CTD-Diver (Eijkelkamp Soil & Water) were used during this study. Compared to fluorescent dyes, the use of NaCl requires larger amounts, which is why density has to be considered. Shafer et al. (2010) observed density effects during their test, but attained mean concentrations of more than 20 g/L after mixing. Lamontagne et al. (2002) conducted several tests and found no density-driven movement while using low concentrations. They suggest to minimize the amount of salt, which leads to negligible density effects, by increasing the EC to a maximum of five times the natural background. Schincariol and Schwartz (1990) and West and Odling (2007) also came to the conclusion that low concentrations show no or only minor density effects.

2.2.2.2 Permeable injection bag method

As an alternative to a hosepipe filled with saline solution, the simplified method for uniform SBDTs uses solid NaCl filled in a permeable bag (e.g. nylon mesh). The bag is attached to a cable or rope and lowered into the GMW or borehole. During up- and downward movement within a selected depth interval or the whole saturated length, the salt dilutes and increases the electrical conductivity (***Figure 5 b***). Using a fine-meshed bag allows dilution but prevents leaks of undissolved salt. By moving the bag at a steady speed, a close-to-uniform distribution of NaCl-concentration can be achieved.

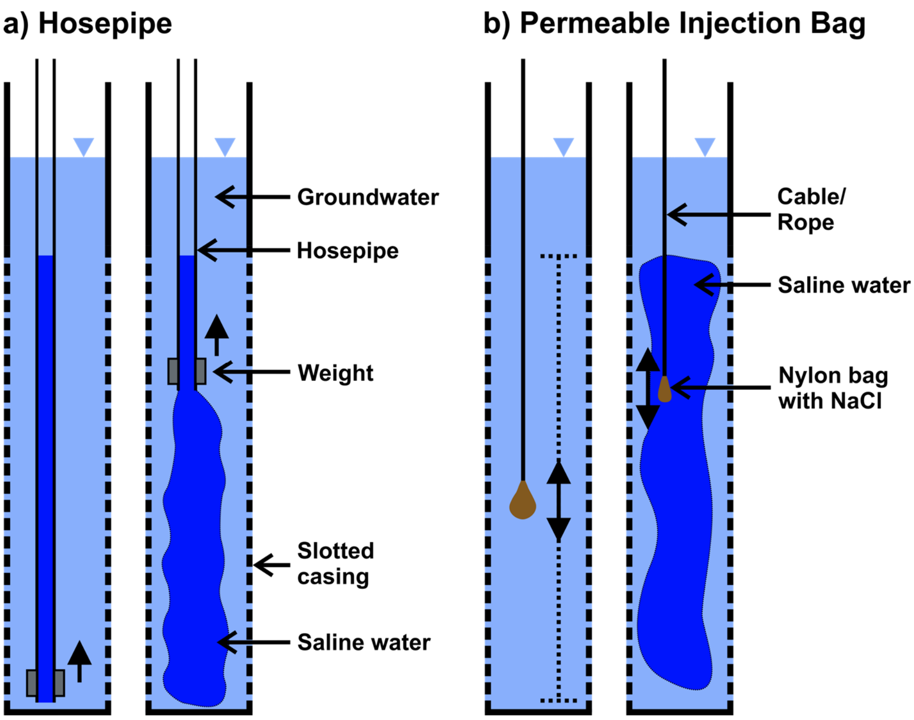

Figure 5: *Illustration of injections using the hosepipe method* ***(a)*** *and the permeable injection bag Method* ***(b)****. Both methods aim at a uniform tracer concentration throughout the saturated zone.*

To prepare an injection, basic information on the GMW or borehole (depth, diameter, water level) and the salt amount (m_{in}) is needed. The latter can be calculated by using Eq. (1):

$$m_{\mathrm{in}} = V\ (\mathrm{EC_b}\ x\ z) \qquad (1).$$

With V being the water volume within the well casing or borehole, $\mathrm{EC_b}$ the mean value of the natural background electrical conductivity, x the factor by which the background EC should be increased, and z the coefficient of a calibration with the used salt and water from the respective field site. During this work, salt amounts between 50 and 900 g were used. Having the calculated salt amount and the water volume within the casing or borehole, an approximation for the expected tracer concentration (c_{Exp}) can be calculated (Eq. 2), with the radius (r) and the saturated length (d_{sat}):

$$c_{\mathrm{Exp}} = \frac{m_{\mathrm{in}}}{\pi\, r^2\, d_{\mathrm{sat}}} \qquad (2).$$

After each measurement, for each depth interval ($d_1 - d_2$), the remaining amount of salt within the casing (m_i) can be calculated with Eq. (3):

$$m_i = \frac{(\mathrm{EC}_{d1} - \mathrm{EC}_{\mathrm{b}d1}) + (\mathrm{EC}_{d2} - \mathrm{EC}_{\mathrm{b}d2})}{2}\ z\ (d_2 - d_1)\ \pi\, r^2 \qquad (3).$$

2.2.3 Filtration velocity

The temporal development of tracer concentration obtained from uniform injections can be used to determine filtration velocities for every depth. The calculation of filtration velocities is based on the dilution versus time relation shown in Eq. (4), which is valid for nonreactive tracers, instantaneous injections and under the assumption that tracer dilution is only caused by horizontal groundwater flow (Freeze and Cherry 1979):

$$\frac{dc}{dt} = -\frac{A\, v_\mathrm{a}\, c}{W} \tag{4}$$

With tracer concentration (c), time (t), cross-section (A), apparent filtration velocity (v_a), and volume of the well segment (W). Rearrangement and integration then leads to Eq. (5) (Pitrak et al. 2007):

$$\ln(c_i) = -\left(\frac{2\, v_\mathrm{a}}{\pi\, r}\right) t_i + \ln(c_1) \tag{5}$$

This can be solved by plotting the natural logarithm of tracer concentration versus time, which shows a linear trend if dilution is only caused by groundwater flow. As a result, Eq. (5) can be reduced to Eq. (6), where m is the slope of the linear trend, which then allows the determination of v_a with Eq. (7) (Piccinini et al. 2016):

$$m = -\left(\frac{2\, v_\mathrm{a}}{\pi\, r}\right) \tag{6}$$

$$v_\mathrm{a} = \frac{m\, \pi\, r}{2} \tag{7}$$

During the linear fitting, the first few concentration values have to be neglected in some cases as they are influenced by mixing effects and dispersion and thus falsify the value of m (Pitrak et al. 2007).

As an alternative to linear regression, apparent filtration velocities can also be determined using the CXTFIT code from the STANMOD software package (Šimůnek et al. 1999). Piccinini et al. (2016) showed, that the apparent filtration velocity can be determined by inversing the 1D advection-dispersion equation. However, instead of using concentration values normalized to C_1, measured tracer concentrations were used as input values. Additionally, CXTFIT also delivers the dispersion for every depth (Piccinini et al. 2016).

The apparent filtration velocity then can be converted into filtration velocity. According to Halevy et al. (1967) v_a consists of filtration velocity (v_f), a correction factor (α) which compensates for the change of flow lines the well or borehole generates, and apparent flow velocities due to density effects (v_k), vertical currents (v_s), vertical mixing (v_m), and molecular diffusion (v_d) (Eq. 8):

$$v_\mathrm{a} = \alpha\, v_\mathrm{f} + v_\mathrm{k} + v_\mathrm{s} + v_\mathrm{m} + v_\mathrm{d} \tag{8}$$

In absence of vertical flow and density effects, and with neglectable influence by diffusion, Eq. (9) results (Halevy et al. 1967; Drost et al. 1968; Piccinini et al. 2016):

$$v_\mathrm{f} = \frac{v_\mathrm{a}}{\propto} \tag{9}$$

The correction factor α (Eq. 10) is calculated with the inner radius of the filter tube (r_1), the outer radius of the filter tube (r_2), the radius of the borehole (r_3) and the permeabilities of filter tube (k_1), gravel filter (k_2) and aquifer (k_3) (Halevy et al. 1967; Drost et al. 1968):

$$\alpha = \frac{8}{\left(1+\frac{k_3}{k_2}\right)\left\{1+\left(\frac{r_1}{r_2}\right)^2+\frac{k_2}{k_1}\left[1-\left(\frac{r_1}{r_2}\right)^2\right]\right\}+\left(1-\frac{k_3}{k_2}\right)\left\{\left(\frac{r_1}{r_3}\right)^2+\left(\frac{r_2}{r_3}\right)^2+\frac{k_2}{k_1}\left[\left(\frac{r_1}{r_3}\right)^2-\left(\frac{r_2}{r_3}\right)^2\right]\right\}} \tag{10}$$

In homogenous gravel aquifers usually $\alpha = 2$ can be assumed (Drost et al. 1968; Hall 1993; Pitrak et al. 2007). In more heterogeneous karst- or fractured aquifers, α can differ at a small scale, depending on the permeabilities of the surrounding rock (Drost et al. 1968).

2.3 Results and Discussion

2.3.1 Permeable Injection bag SBDTs

Using the PIB method, 34 dilution tests were carried out in different depth ranges and under varying conditions. The deepest GMW had a saturated length of 52 m and a total depth of 122 m, while the shallowest GMW had 5 m of saturated length and a total depth of 8.5 m. In eight GMWs, more than one SBDT was performed to confirm the results and check reproducibility. All tested GMWs are equipped with slotted casing, however, all major flowing features could be identified for each well. Due to the effect of filter gravel and slotted casing, it cannot be ruled out that not all smaller flowing features were detected. ***Table 3*** shows the results of selected SBDTs carried out in karst and alluvial GMWs during this work using different injection methods. To avoid density effects, all tests aimed at increasing the background conductivity by a factor of 3 – 5 or 1,000 – 2,000 µS/cm, which corresponds to concentrations of 2 – 3 g/L NaCl.

Table 3: *Summary of selected SBDTs in the karst aquifer (GMW 7733, 7721, 7313, 7939) and the alluvial aquifer (GWM 5303, 5304, 5312). PIB permeable injection bag; HP hosepipe; n.d. not determined.*

GMW-No.	Water Level below surface (Saturated Length) [m]	Date	Injection Method	Number of EC profiles	Duration [h]	Half-time [h]	Max. (Mean) App. filtration Velocity [m/h]	Vertical Flow
7733	26.11 (13.89)	05.09.16	PIB	9	22.5	0.78	0.21 (0.09)	no
	26.49 (13.51)	07.04.17	PIB	16	23.0	0.63	0.24 (0.10)	no
	26.21 (13.79)	14.08.18	PIB	27	22.1	0.83	0.23 (0.09)	no
	26.58 (13.42)	08.07.19	PIB	19	22.9	0.70	0.23 (0.10)	no
	26.59 (13.41)	09.07.19	PIB	18	12.1	0.65	0.24 (0.10)	no
7721	22.9 (51.1)	06.09.16	PIB	7	22.4	2.73	n.d.	yes
	25.4 (48.6)	12.04.17	PIB	13	22.4	0.48	n.d.	yes
	25.8 (48.2)	17.10.18	PIB	20	21.1	1.12	n.d.	yes
	26.01 (47.99)	10.07.19	PIB	15	23.6	1.32	n.d.	yes
	26.01 (47.99)	11.07.19	PIB	12	9.1	1.50	n.d.	yes
7313	59.40 (14.35)	07.09.16	PIB	10	1039.1	8	0.05 (0.01)	no
	65.27 (8.48)	12.07.17	PIB	27	820.5	111	0.04 (-)	no
7939	8.40 (20.60)	14.08.18	PIB	16	379	44	0.01 (-)	no
5303	7.68 (8.32)	21.08.19	PIB	16	3.6	0.17	n.d.	yes
	7.78 (8.22)	29.08.18	HP	11	1.4	0.23	n.d.	yes
5304	6.58 (6.42)	31.07.17	PIB	15	4.2	0.48	n.d.	yes
	6.68 (6.32)	16.08.17	HP	14	7.1	0.35	n.d.	yes
	6.95 (6.05)	15.08.18	PIB	24	6.1	1.40	n.d.	yes
5312	7.24 (8.51)	19.07.17	HP	12	2.4	0.43	n.d.	yes
	7.24 (8.51)	20.07.17	PIB	12	3.2	0.92	n.d.	yes
	7.40 (8.35)	02.08.18	PIB	18	2.9	0.55	n.d.	yes
	7.53 (8.22)	24.08.18	PIB	16	2.9	0.65	n.d.	yes

Figure 6 shows the results of a SBDT in karst GMW 7733, using the PIB method. This monitoring well has a depth of 40 m (all depths refer to the respective well cap) and the water level was at 26.59 m. For this test, 200 g of NaCl were used, enough to increase the natural EC by almost five times. With Eq. (2) the estimated concentration was calculated (1,215 mg/L, dashed red line). The injection took 8 min, and was followed by an immediate measurement of an EC-profile. As can be seen in ***Figure 6 a***, the estimated NaCl-concentration is obtained only in the lower section of the GMW, while there is a significantly lower concentration in the upper part. This indicates a higher groundwater flow within the first meters and not an uneven injection, which would have resulted in concentrations above the expected value in other sections of the water column.

The fast decline in the upper part continues in the following measurements and is followed by a slower decrease between 31 and 35 m. Around 36.5 m, another zone with a slightly higher decrease suggests a flowing feature with higher groundwater flow. Near the bottom, the slowest decline of tracer concentration was observed. Altogether, the tracer amount decreases quickly, so that only very low tracer concentrations are measured 12 h after the injection, which indicates a good connection to the karst aquifer and the conduit system. GMW 7733 is one of the monitoring wells with the fastest outflow compared to other karst GMWs; the longest test in GMW 7313 took more than 6 weeks (***Table 3***).

In ***Figure 6 b***, all EC-profiles are normalized by dividing each profile by the first measurement, to show the percentage decline of NaCl concentration for each depth. Normalized graphs are useful to compensate for uneven injections and ensure a better visualization of flowing features. In this case, both figures indicate the highest outflow around 29 m. In this depth, the geology, obtained from the drilling log, shows a change of lithology from silty limestone to pure limestone. This chance of facies very likely favored karstification and the development of a preferential flow horizon.

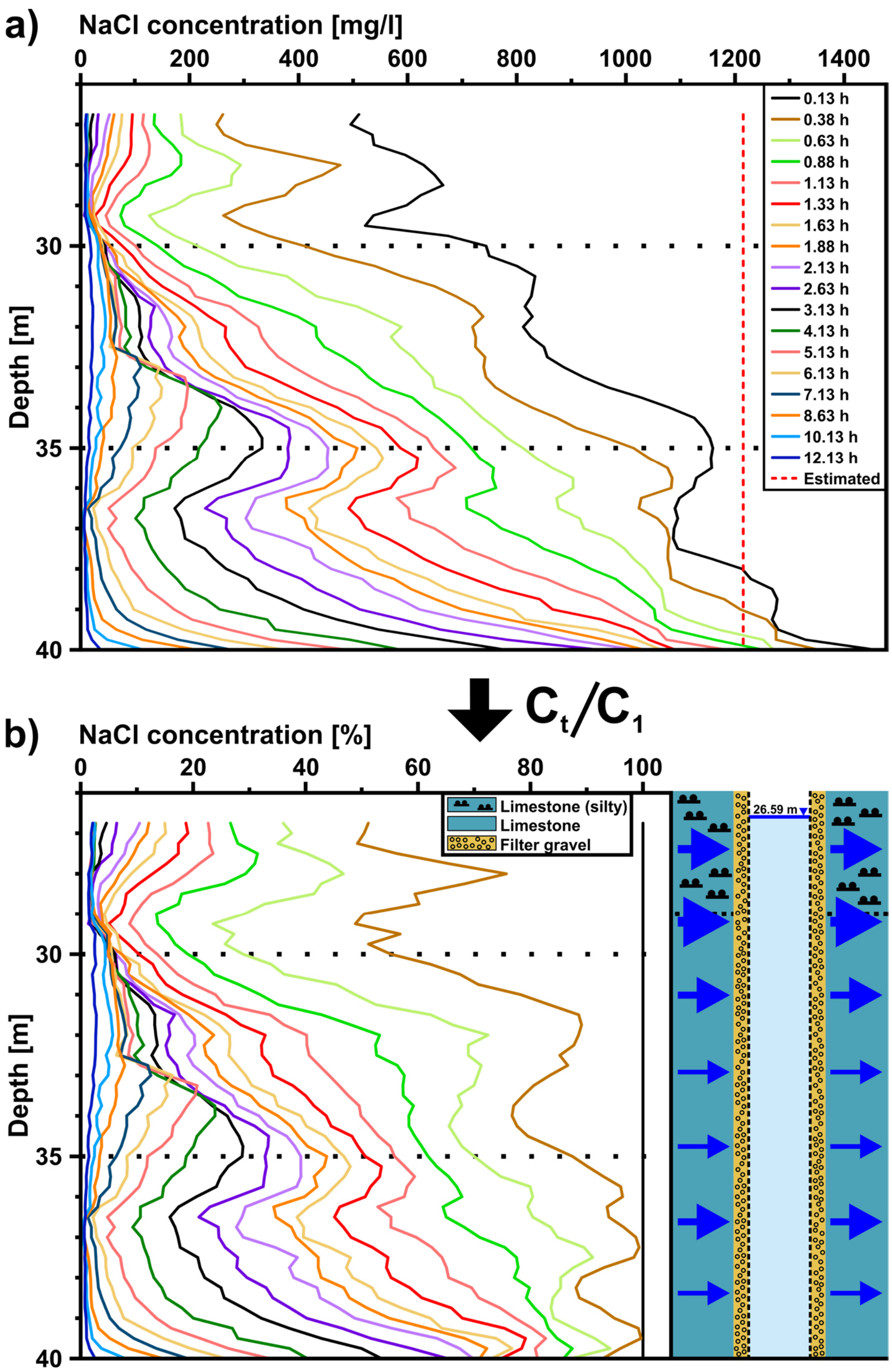

__Figure 6:__ Results of a SBDT using the PIB method in GMW 7733 (09.07.2019) including geology and identified outflow behavior. __(a)__ Absolute values in mg/L; __(b)__ normalized by dividing each profile by the first profile.

For all tests the start of the injection was used as t_0, since outflow processes start immediately and so the first EC profile is already influenced by groundwater flow and an undisturbed injection profile is just hypothetical. ***Figure 7*** shows the timeline of the SBDT in GMW 7733 on 09.07.2019. The first measurement (t_1) always started directly after the injection. The first EC profiles were measured every 15 min; later on, the intervals were increased to 2 h in four steps.

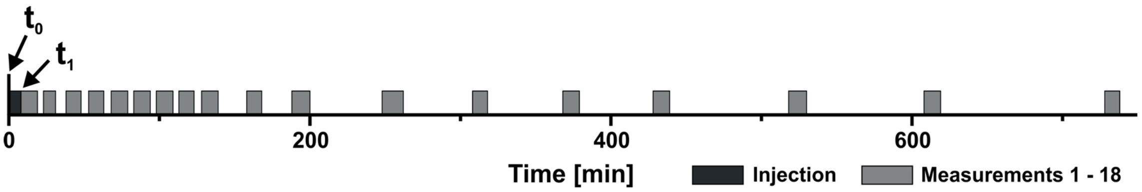

Figure 7: *Timeline of the SBDT in GMW 7733 on 09.07.2019. A total of 18 EC profiles were measured; one measurement took between 8 and 14 min (average 11 min).*

SBDT results from a karst monitoring well with vertical flow are shown in ***Figure 8 a***. GMW 7721 has a total depth of 74 m. On 06.09.2016, the water level was at 22.9 m, resulting in a saturated length of 51.1 m. Due to the depth, 875 g of NaCl was injected using the permeable injection bag method. The first profile shows a maximum concentration at 33 m, indicating a nonperfect injection. However, flowing processes could still be observed and interpreted. It is noticeable that between measurements number 2 and 6, maximum concentrations are almost constant and the shape of the curves is very similar, but with a steady downward offset. The missing decrease of NaCl concentrations in the middle part indicates missing horizontal outflow in the section between 40 and 70 m. The vertical offset of concentration-profiles with little changes regarding the shape is a sign of vertical flow within the GMW. Using the vertical offset and time differences between the measurements, the vertical velocity can be estimated at 5.5 m/h. No tracer accumulation near the bottom is observed, indicating an outflow horizon at approximately 72 m. This results in the interpreted flow paths shown in **Figure 8 a**. Twenty-two hours after injection, the salt plume reaches the bottom, signifying that GMW 7721 also has a good connection to the fracture and conduit network, resulting in fast tracer outflow.

GMW 7721 was cleaned with hydraulic pulsing on 11.04.2017, which removed black deposits in casing and filter gravel. ***Figure 8 b*** shows the results of a dilution test conducted 1 day after the cleaning. NaCl concentrations decrease over the whole saturated length caused by horizontal flow, which is no longer blocked by deposits. Also, vertical flow is substantially lower, and between 70 and 74 m, almost no decrease of tracer concentration is observed. During the cleaning, some of the deposits were not removed but sank to the bottom, where they partially block the outflow near the bottom leading to a weaker vertical flow component. Also, the water level during the second SBDT was 2.5 m lower, which leads to smaller hydraulic head differences and therefore less vertical flow.

In addition to the newly occurring horizontal flow, success of the cleaning can also be confirmed with the determined half-time, the time span until 50% of tracer has flowed out of the respective GMW. Before the cleaning, it took 2.7 h until the salt amount in the water column was half of the injected amount, afterwards only 0.5 h. These results were confirmed by another four SBDTs in GMW 7721. However, 16 months after the cleaning, half-time increased again to 1.1 h and, after 25 months, to 1.3–1.5 h (***Table 3***), which indicates new deposits in the filter gravel or the slotted casing. These results show that the permeable injection bag method can also be used to check the effects of well cleaning.

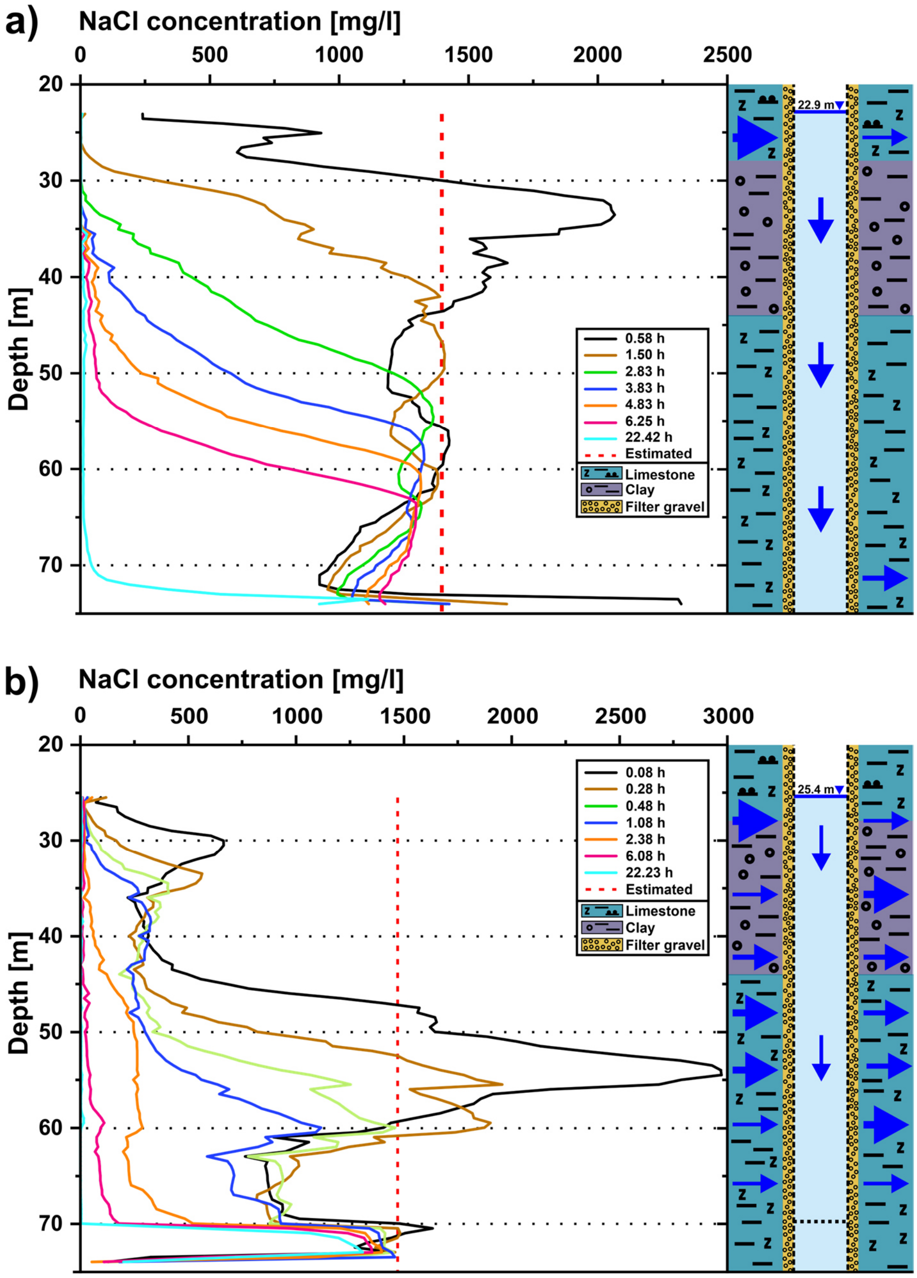

Figure 8: *Results of two SBDTs with the PIB method in GMW 7721.* ***(a)*** *Before cleaning, which shows that the monitoring well displayed a strong downward movement without significant decrease of the maximum value from measurements 2 – 6, which suggests vertical flow (06.09.2016).* ***(b)*** *After the cleaning on 11.04.2017, which shows that a complex combination of vertical flow and newly enabled horizontal flow can be derived from the concentration profiles (12.04.17).*

For all uniform injections, the tracer amount within the casing was calculated for each measurement using the concentrations from each depth (Eq. 3). This allows a characterization of the overall behavior of the well and also a better comparison of different sites. ***Figure 9*** displays the decline of NaCl amount for all tested GMWs. Half-times vary between 1 and ~1,000 h, confirming major differences in groundwater flow in the study site. GMWs in the alluvium aquifer tend to show a faster outflow than GMWs in the karst aquifer, but individual karst GMWs have a good connection to the conduit system, and thus also possess a rapid decline. In contrast, some karst GMWs show a weak and long-lasting decrease indicating slow advection (***Table 3***).

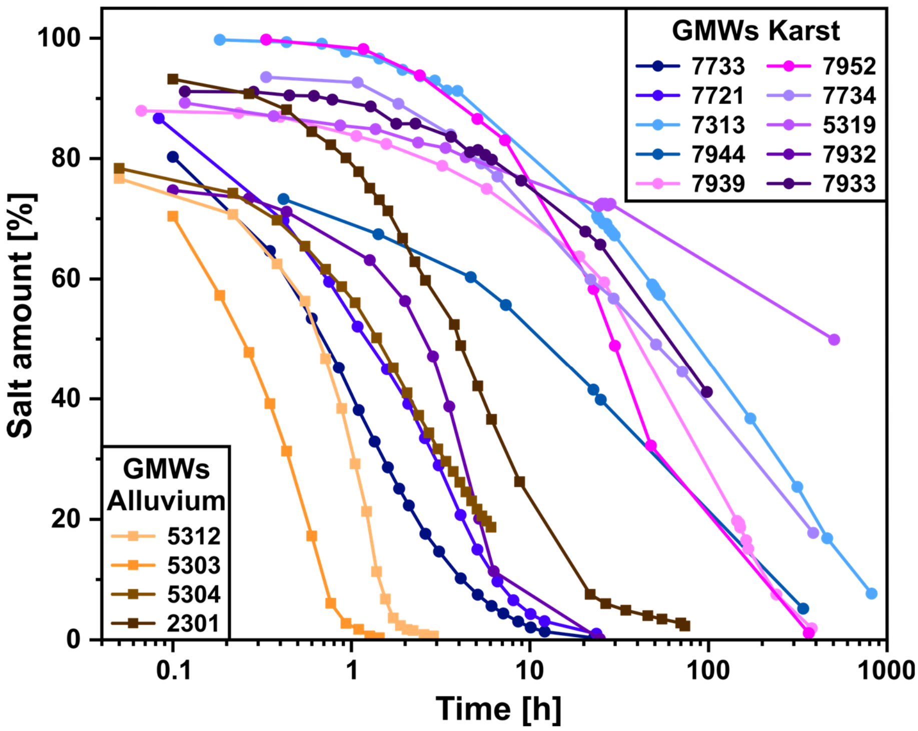

Figure 9: *Development of salt amount with regard to the injection amount for each tested GMW in karst and alluvium. For the eight monitoring wells with multiple SBDT-results, just one curve is shown.*

2.3.1.1 Reproducibility

The reproducibility of the permeable injection bag method was examined based on two aspects, the temporal development of salt amount and apparent filtration velocities. Repeated tests in several GMWs, conducted under similar hydraulic conditions, were compared with regard to the decrease of salt amount in the well. ***Figure 10*** shows salt amount versus time for 14 SBDTs in three different monitoring wells. The three GMWs are clearly separated from each other, while curves from the same site are almost identical and thus are a strong indicator for the reproducibility of the PIB method. Small differences can be explained with changing injection times due to different salt amounts, varying grain sizes, and slight changes in the water levels. Since GWMs 7733 (karst) and 5303 (alluvial) both include one SBDT with the hosepipe method, these results also indicate the reproducibility of SBDTs in general, irrespective of the injection method used.

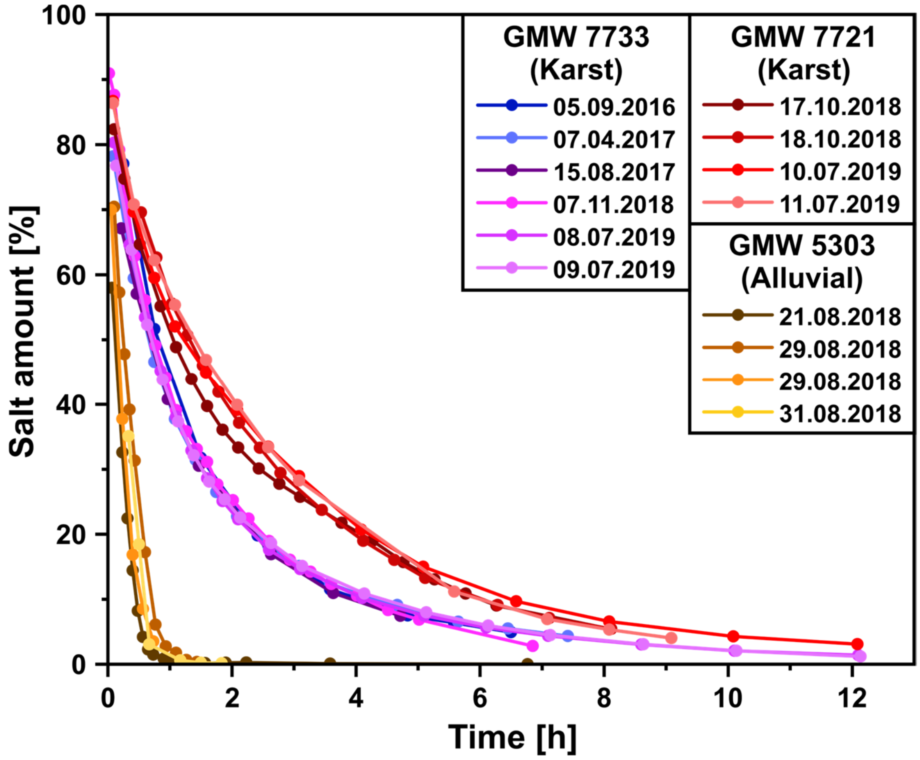

Figure 10: *Development of salt amount for repeated SBDTs in GMW 7733 (n = 6), GMW 7721 (n = 4), and GMW 5303 (n = 4) conducted under similar water levels. GMW 7733 (15.08.17) and GMW 5303 (29.08.2018) each include one SBDT with the hosepipe method. The conformity for each GMW demonstrates the reproducibility of SBDTs and especially the permeable injection bag method.*

Moreover, reproducibility was assessed by comparing velocities of repeated tests in GMW 7733, which shows no vertical flow and thus allows the calculation of apparent filtration velocities (v_a) with both methods described in section 2.2.3. Due to missing permeability values of the surrounding limestone, the correction factor α (Eq. 10) could not be calculated and thus also no filtration velocities (v_f). Still, the comparison of the different SBDTs is possible with the determined v_a-values.

Figure 11 shows the mean apparent filtration velocities and the standard deviation for each depth gained from six SBDTs in GMW 7733 between 09/2016 and 07/2019 under similar hydraulic conditions. Both methods produced similar velocity profiles for each test, resulting in a low standard deviation, which also proves the reproducibility of the PIB method. A comparison of the two methods of determination shows a good accordance. Plotting filtration velocities obtained from CXTFIT versus filtration velocities from linear regression results in $R^2 = 0.996$ and $a = 1.009$. With these minor differences, both methods are applicable for analyzing uniform SBDTs. One advantage of CXTFIT, however, is that it is not affected by personal valuation. Regardless of which method is chosen for the processing of SBDT-data, verifications using the other method are recommended.

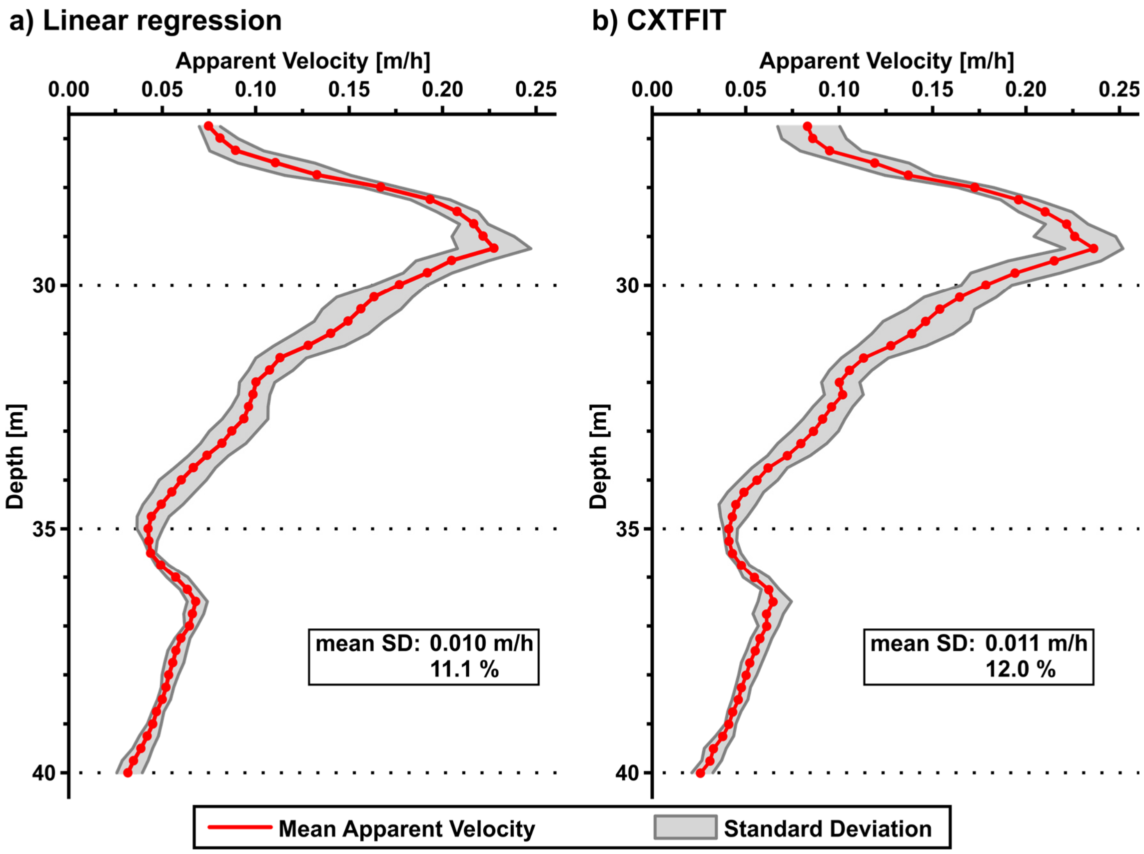

Figure 11: *Mean apparent filtration velocity from six SBDTs in GMW 7733 with standard deviation.* ***(a)*** *Results obtained from linear regression.* ***(b)*** *Results obtained from CXTFIT. For both determination methods, the results show only slight deviations, indicating good reproducibility.*

2.3.2 Comparison of injection methods

Results show that SBDTs, and especially the two used injection methods, produce significant results and contribute to the understanding of flow processes in GMWs or even whole aquifers. Although both uniform injection methods deliver the same results, the performance must be assessed in more detail (***Table 4***). Due to the dilution process, an injection with the PIB takes more time compared to the hosepipe method; however, grinding the salt in advance and minimizing the amount of tracer helps to reduce the dilution time.

Using a hosepipe for uniform injections, usually leads to a more homogeneous tracer concentration over the whole length compared to the PIB, which sometimes produces uneven EC profiles, due to unsteady movement during the dilution process. However, normalizing the data to the first measurement equalizes uneven profiles without losing any information. Using a PIB for the injection reduces the effort of SBDTs significantly and is less time consuming including the preparation. Especially for deep GMWs or boreholes, the hosepipe method requires several tens of liters of tracer solution, which must be prepared and transported to the test site. Furthermore, deep GMWs or boreholes require long hosepipes and, due to their weight, at least two persons or the use of a cable winch.

For multiple GMWs or boreholes with different depths, several hosepipes are needed, otherwise the handling gets very complicated. In contrast, the PIB method demands less preparation and is more flexible, since the permeable bag as well as the cable can be used for several tests and different depth ranges. Also, the handling during the injection is easier and can easily be done by one person.

Table 4: *Rating of the injection methods based on field experiences and results (++ very good; + good; 0 neutral; - deficient).*

Performance criterion	Hosepipe method	Permeable injection bag method
Required personnel	0	++
Preparation time	+	++
Duration of Injection	++	+
Flexibility (depth range)	-	++
Deep GMWs or boreholes	-	++
Handling	+	++
Homogeneous injection	++	+
Costs	+	++

2.4 Conclusions

Compared to other methods such as pumping tests or flowmeter measurements, SBDTs need less equipment and require less effort. Especially, the simplified PIB method is easy to conduct, even by a single person, and only uses commonly available materials, which altogether minimizes costs. However, still meaningful and valuable conclusions about monitoring wells and aquifer properties can be gained, making this method suitable also for low-income countries, projects with limited resources, and study areas with a large number of monitoring wells. Results during this work also demonstrated the reproducibility and flexibility of the simplified method. The PIB method is especially applicable for deep GMWs and difficult accessible testing locations, since no heavy equipment is needed. Further conclusions are:

- The first SBDT in a GMW or borehole should be a uniform injection, since it delivers results for the entire saturated length and leads to a basic understanding of in- or outflow. The injection method should be chosen depending on the depth and the accessibility.
- Results show that increasing the natural background conductivity by a factor of 3 – 5, or 1,000 – 2,000 µS/cm, which in this case corresponds to a maximum of 2 – 3 g/L NaCl in the water column, is sufficiently high to identify flowing features. Also, similar to Lamontagne et al. (2002), no density effects were observed within these limits. In general, tracer use should be minimized to avoid impacts on natural flow conditions and density affecting the interpretation.

- Normalized graphs compensate unequal injections and can be used to separate effects caused by flowing features from methodical influences. Normalizing concentration profiles helps to compare multiple SBDTs conducted in the same GMW or borehole; however, it is not suitable for dominant vertical flow.
- In the absence of vertical flow, both injection methods can be used to calculate horizontal flow within wells or boreholes. For the determination of filtration velocities, both linear regression and CXTFIT provide good results; cross-validation of individual values can be used for verification. Since the determination of the correction factor α, used to convert apparent filtration velocities to filtration velocities, is often not possible due to unknown permeabilities, the apparent filtration velocity can be used to compare different GMWs.
- Despite being conducted in boreholes equipped with slotted casing, all SBDTs could identify the major flowing features in the tested wells.
- SBDTs in the karst aquifer showed the expected wide range of results, with test durations between several hours and multiple weeks. Also, the heterogeneity within each well, e.g. outflow horizons next to inactive segments, could be shown nicely, making SBDTs especially interesting in karst aquifers. In contrast, GMWs in the alluvial aquifer show a more homogeneous behavior and no abrupt changes within the profiles.

Acknowledgments

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CHAPTER 3

3 A novel probe for point injections in groundwater monitoring wells

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A patent application has been filed for the point injection probe developed in this study.

Abstract

Groundwater monitoring wells or boreholes often show complex flow behaviors that are essential to understand for the characterization of aquifer systems. In karst or fractured aquifers, where complex conduit and/or fracture networks with differing hydraulic heads can be intersected by a well or borehole, vertical flow is highly probable. Single-borehole dilution tests (SBDT) with uniform injections are, in general, a good method to gain knowledge about a specific well or borehole, but tend to deliver ambiguous results regarding vertical flow, while SBDTs with point injections are an effective method to identify vertical flow.

This technical note introduces a newly developed probe for point injections in groundwater without disturbing the natural flow field. In order to evaluate this probe, several tests were conducted in the laboratory and in groundwater monitoring wells that show vertical flow. During repeated tests in the laboratory, the new point injection probe showed a good reproducibility regarding the shape and extent of the tracer cloud after an injection. The opening mechanism was found to be well-functioning and reliable. Field tests lead to significant results for all tested wells and showed that the probe can easily be operated by a single person. Due to the flexibility regarding tracer, aquifer and injection depth, combined with the easy handling, it is a useful device, suitable for the investigation of boreholes and groundwater monitoring wells, and a good alternative to existing methods.

3.1 Introduction

In-situ characterization of groundwater flow is important for the understanding of complex aquifer systems. A wide range of geophysical, hydraulic and tracer-based methods is available to examine aquifer properties and groundwater flow directly in the aquifer. For the investigation of flow systems in boreholes or groundwater monitoring wells (GMW) distributed temperature sensing has been widely used in the last years (Leaf et al. 2012; Banks et al. 2014; Read et al. 2014; Sellwood et al. 2015; Bense et al. 2016). One other efficient and practicable method that delivers important and useful results about groundwater flow are single-borehole dilution tests (SBDTs). Uniform tracer injections throughout the entire saturated length deliver information about the entire groundwater monitoring well or borehole and can be achieved with several methods, for example by the use of hosepipes, often combined with pumping (Hall 1993; West and Odling 2007; Shafer et al. 2010; Maurice et al. 2011; Libby and Robbins 2014). Alternatively, the new method introduced by Fahrmeier et al. (2021), which uses a permeable injection bag, can be used.

The results of uniform injections for one particular depth are not always representative for the entire borehole, and vertical flow components are not always identifiable. In these cases, point injections can be used to complete the information gained by uniform injections, whereby the results of the uniform injection can be used to determine the depth for a point injection (Maurice et al. 2011). Information about vertical flow is important for the understanding of the processes within boreholes or GMWs and can also contribute to the understanding of complex aquifer systems. Especially karst and fractured aquifers often show vertical flow, due to the compensation of different pressures in solutionally enlarged fractures and bedding planes that are intersected by the boreholes or GMWs (Michalski and Klepp 1990). Additional to information about vertical flow, point injections can also be used for the characterization of one specific depth, if the productivity or flow rate of this depth is of particular interest.

Common methods for characterizing a specific depth in a borehole or GMW use systems with two packers that enclose a depth interval which then can be tested. Most of these systems inject the respective tracer directly in the test chamber, where it is continuously mixed, either using a pump or a mixing unit (e.g. a propeller), and also directly measured with a measuring device placed in the test chamber (Drost et al. 1968; Grisak et al. 1977; Palmer 1993; Novakowski et al. 2006; Gouze et al. 2008; Yang et al. 2019; Devlin 2020). A modified version continuously circulates water from the interval between the packers to the surface and back. During this circulation, the tracer is added and afterwards the concentration is monitored with an in-line device (Jamin et al. 2015).

Other point injection methods, without the use of packers, deliver results for the whole well or borehole. Poulsen et al. (2019b) use a continuous injection of tracer in one specific depth, combined with pumping near the top of the well. This allows one to draw conclusions on all flowing features between injection and extraction depth. Related methods were used by Brouyère et al. (2008), Leaf et al. (2012) and Read et al. (2015). However, due to the pumping, natural vertical flow is not visible or at least strongly influenced.

All these methods are not suitable to investigate and characterize the natural in- and outflow behavior of GMWs or boreholes completely, since they affect the natural flow system due to pumping or blocking vertical flow with hydraulic packers. If vertical flow is to be taken into account, a point injection under natural gradient conditions, without pumping influences or packers, is necessary. Injecting tracer under natural-gradient conditions reveals vertical flow by an up- or downward movement of the tracer plume. ***Figure 12*** shows typical movements of a tracer plume after a point injection under natural conditions, depending on the water movement within the well or borehole. ***Figure 12 a*** displays a well with downward flow and one outflow zone near the bottom, and ***Figure 12 b*** shows upward flow in combination with a single outflow zone near the top. ***Figure 12 c*** shows downward flow in combination with horizontal flow, which leads to a faster reduction of the tracer in the well. ***Figure 12 d*** displays a well without any vertical flow but a horizontal outflow at the depth of the tracer cloud. In this case, the tracer plume remains at the injection depth and the peak just widens a little, due to diffusion.

Different devices can be used to achieve a point injection under natural flow conditions. Pitrak et al. (2007) used a specially-designed tool consisting of a thin plastic hose connecting two syringes with a volume of 20 mL; one is kept at the surface, the other one is lowered into the selected depth. Pushing the first syringe leads to a release of the tracer from the second syringe. Tate et al. (1970) introduced an injector with a cylindrical container and an electromagnetic opening mechanism. When this mechanism is triggered, the outer part of the container sinks down and releases the tracer into the groundwater.

This Technical Note introduces a newly developed probe for point injections in groundwater, without disturbing the natural flow or preventing vertical flow components. In order to evaluate the point injection probe, several tests were conducted in the laboratory and in groundwater monitoring wells that show vertical flow.

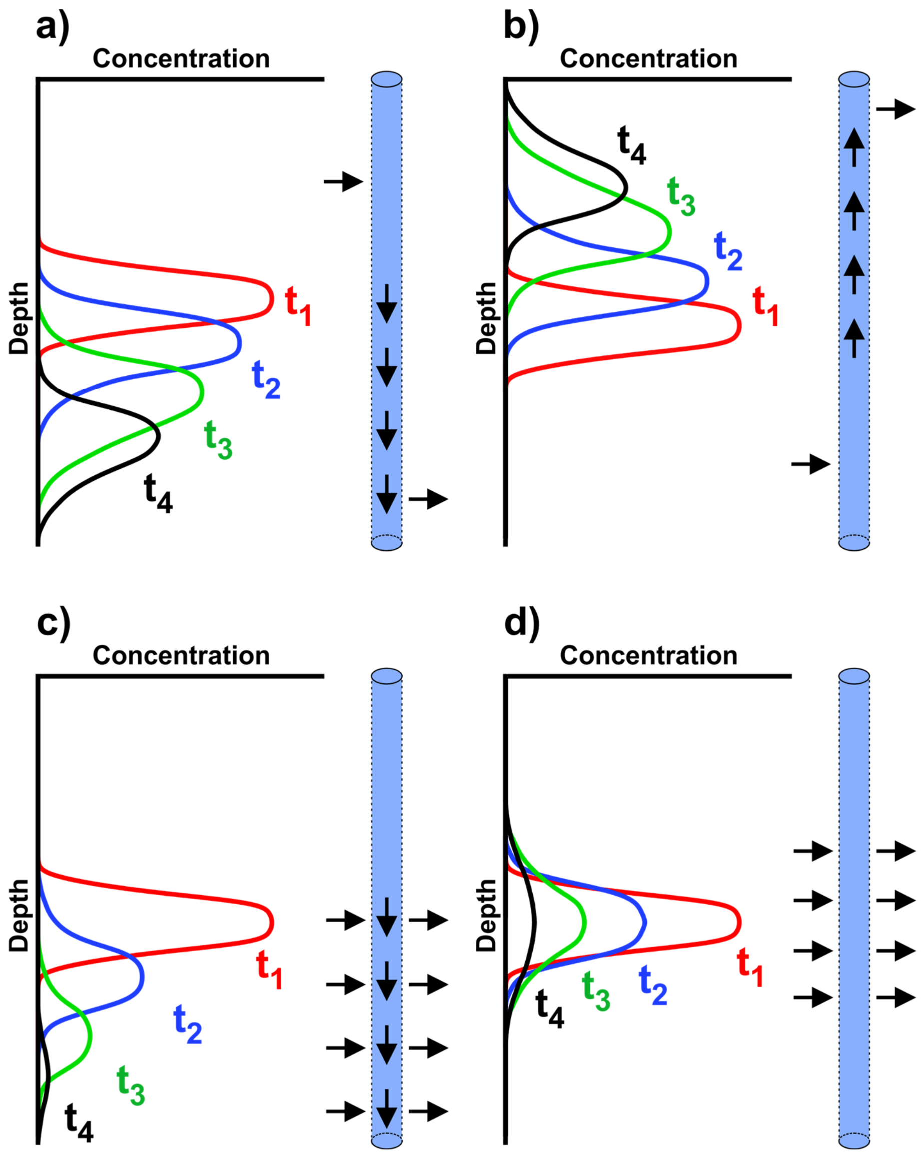

Figure 12: *Four typical concentration patterns after point injections in groundwater monitoring wells. Curve t1 shows the ideal salt plume after the injection, and t2, t3 and t4 show the development of the salt plume at increasing times, induced by groundwater flow in the well.*

3.2 Point injection probe

The concept of the new point injection probe is based on depth-dependent sampling devices which are opened or closed by a falling weight. Based on this idea, and in cooperation with a precision engineer, the injection probe was designed. It consists of a container with a movable outer casing and a mechanical opening mechanism on top. It is attached to a measuring tape, along which a falling weight is dropped down to trigger the opening mechanism. ***Figure 13*** shows pictures of the probe in closed and opened state. The container is held together by three hooks, fixed by a rubber band. When the trigger cone is pushed down, it overcomes the strength of the rubber band, causing the hooks to unlock the container's casing, which then slides down and releases the tracer in the surrounding groundwater (***Figure 14 a***).

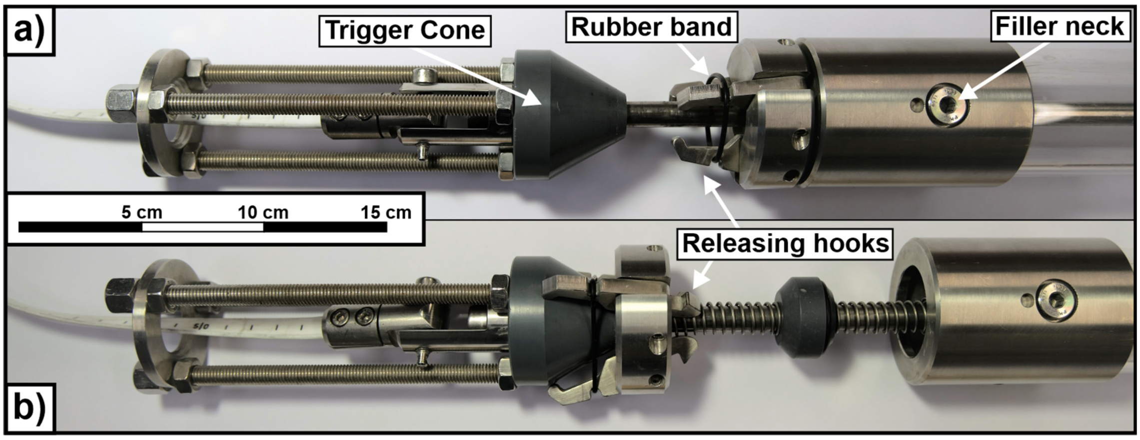

Figure 13: *Detailed view of the* ***(a)*** *closed and* ***(b)*** *opened injection probe. When the trigger cone is pushed down, it opens the three hooks, which allows the casing to slide down.*

With the help of a funnel, the probe can be filled with tracer solution through the filler neck near the top. The probe can be used with any kind of soluble tracer, e.g. NaCl or fluorescence dyes. The container was configured with a capacity of 500 mL, a length of 50 cm and a diameter of 6 cm. Due to the small diameter, the point injection probe can be used in all wells or boreholes with a diameter larger than 3 inches (7.6 cm).

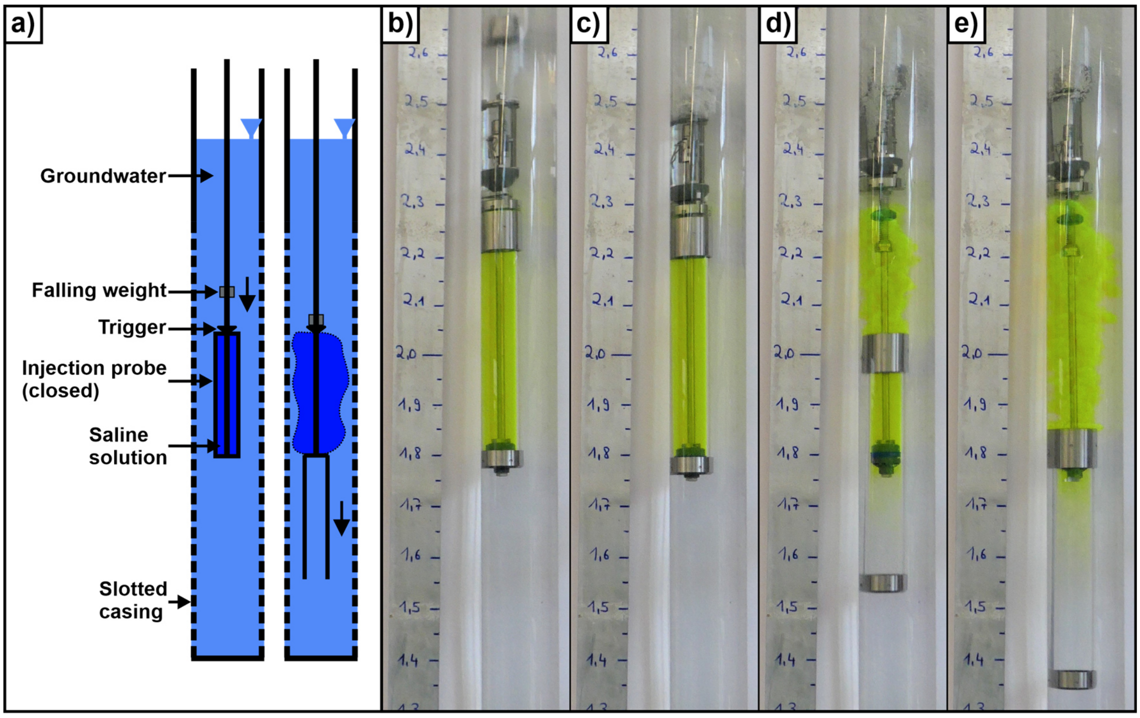

Figure 14: ***(a)*** *Illustration of a point injection using the new probe;* ***(b)*** *–* ***(e)*** *pictures of an injection using uranine in the acrylic glass well in the laboratory:* ***(b)*** *shows the closed probe directly before the falling weight hits the mechanism,* ***(c)*** *is in the exact moment when the opening mechanism is triggered; in picture* ***(d)*** *the probe is already halfway open, and* ***(e)*** *shows the completely opened probe.*

Figure 14 shows the probe during an injection in the laboratory using uranine for better visibility. ***Figure 14 b*** shows the closed probe immediately before the weight hits the opening mechanism;

Figure 14 c displays the exact moment the opening mechanism is triggered; ***Figure 14 d*** shows the casing dropping down and releasing the tracer into the surrounding water; the final stage of the injection with the completely opened probe can be seen in ***Figure 14 e***. The entire opening process takes around 1.5 seconds.

3.3 Test sites

The new point injection probe was tested under laboratory conditions, as well as in groundwater monitoring wells in the field. The laboratory experiments were conducted in a transparent acrylic glass tube with a length of 6 m. The tube was filled with water and used for several injections, to test the probe under perfectly-controlled no-flow conditions and to check the injection mechanism visually. Field tests were conducted in the groundwater protection area of a large water supplier in South Germany (***Figure 15***), which contains a complex aquifer system and was already investigated with a large-scale multi-tracer test and several SBDTs (Fahrmeier et al. 2021). The combination of the large karst aquifer with the overlying gravel aquifer leads to vertical flow in several groundwater monitoring wells. Since both downward and upward flows occur, this area was chosen for the field tests of the new probe.

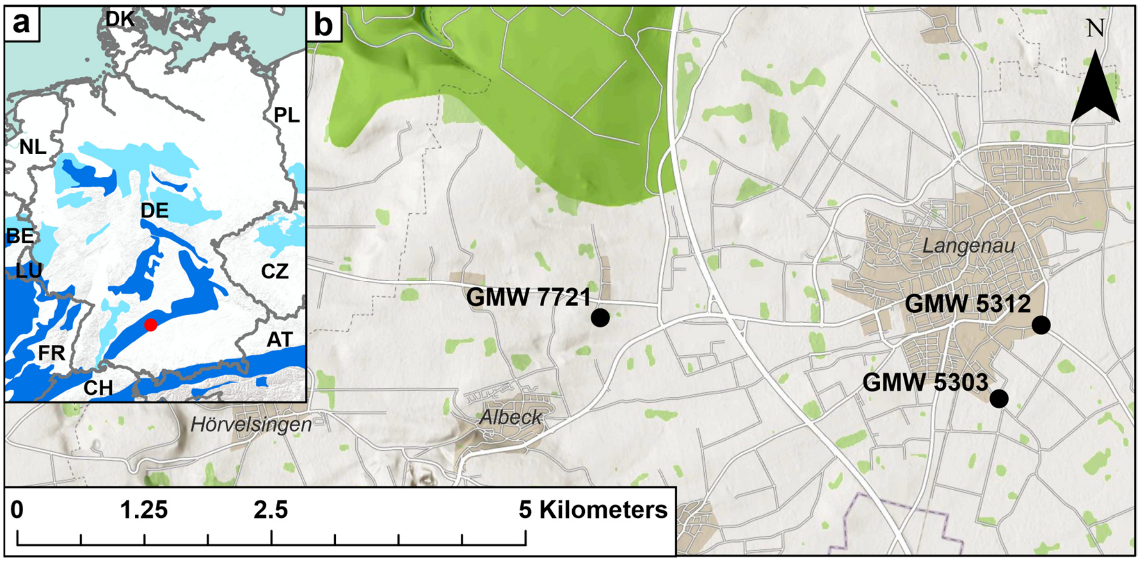

Figure 15: (a) *Location of the study site shown on a cut-out of the World Karst Aquifer Map (WOKAM, Chen et al. 2017; dark blue: continuous carbonate rocks, light blue: discontinuous carbonate rocks; country codes from International Organization for Standardization 2023).* ***(b)*** *Locations of the three groundwater monitoring wells (GMWs) used for the evaluation of the point injection probe.*

3.4 Results and Discussion

3.4.1 Laboratory tests

To check and evaluate the point injection probe under completely undisturbed conditions, repeated tests were conducted in the acrylic glass tube in the laboratory. Based on the observation of these tests, it was possible to make some adjustments for a better functionality of the opening mechanism. Since the acrylic glass tube has no outflows or vertical flows, injections at the same depth using the same tracer quantity should ideally result in identical concentration profiles. Knowing the shape of the injection curve allows a correct interpretation of the movement of the tracer plume as well as clarification as to whether vertical flow is present or not. It is also important for the comparison of different tests. ***Figure 16*** shows profiles of NaCl concentrations measured directly after the injections using an electrical conductivity meter (TLC Meter Model 107, Solinst Ltd, accuracy of 5 % or 100 µS/cm). During measurements, in the laboratory as well as in the field, the TLC Meter was moved carefully while avoiding sudden and fast movements to minimize mixing within the well. With a relation of cross-section areas of 1:50 to 1:70, the impact on the natural water flow is negligible.

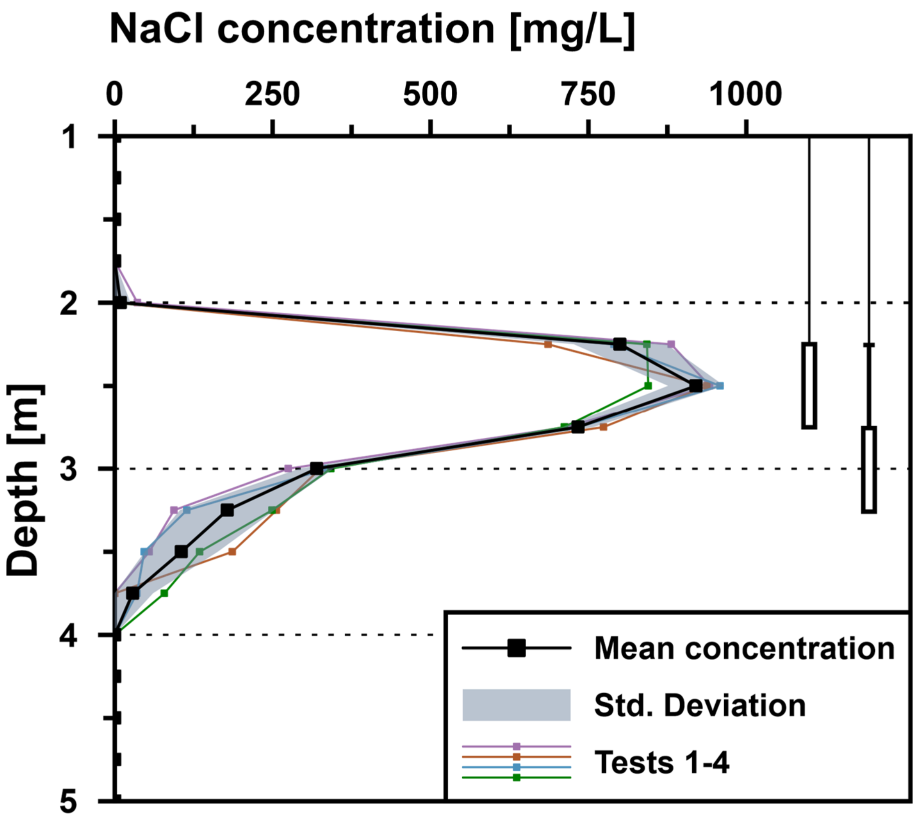

Figure 16: *Concentration profiles of repeated point injections under laboratory conditions, measured immediately after tracer release. For each injection, the probe was filled with 500 mL of a 25 g/L NaCl-solution. The standard deviation of the four profiles between 2 m and 3.75 m is 11 %, while the accuracy of the TLS Meter is at 5 %. On the right side, the depths of the closed and opened probe are indicated.*

The resulting curves show a high conformity and a standard deviation of 44 mg/L from the mean value, indicating that the probe always creates the same injection profile under undisturbed conditions, which is essential for further use. For a further evaluation, R^2 and RMSE were calculated for each pair of injection profiles, resulting in mean values of 0.9734 and 45.6, respectively. As intended, the highest tracer concentration was always measured at the depth where the middle of the closed probe was placed. The salt plume extends vertically about 1.5 to

1.75 m for each test, which still can be considered as a point injection, especially in deep wells. The asymmetry in the lower part might be induced by the downward movement of the container, as well as by the movement of the electrical conductivity meter during the measurement.

3.4.2 Field tests

After the tests in the acrylic glass tube, the point injection probe was used for point injections in three groundwater monitoring wells on the Swabian Alb, where previous research has revealed vertical flow (Fahrmeier et al. 2021). Measurement intervals for each GMW where chosen based on the movement of the salt plume and adapted during the tests. ***Figure 17 a*** shows a contour plot of a SBDT in GMW 5312, where 12.5 g NaCl (500 mL of 25 g/L solution) were injected at a depth of 14 m (all depths refer to the respective well cap; injection depths indicate the depth of the middle of the closed probe). The black squares indicate the center of the salt plume for each measurement.

At the first measurement, the salt plume extends about 2.5 m (***Figure 17 b***), which is larger than during the tests in the laboratory. This is caused by vertical flow, which is demonstrated by the next measurements that show a clear upward movement of the salt plume. Based on the vertical offset between the maximum concentrations for each measurement, or alternatively based on the offset of the center of the tracer cloud, the vertical upward flow can be estimated at around 1.5 m/h. Directly from the beginning, the salt amount shows a rapid decrease, which indicates an additional horizontal flow in the lower part of GMW 5312.

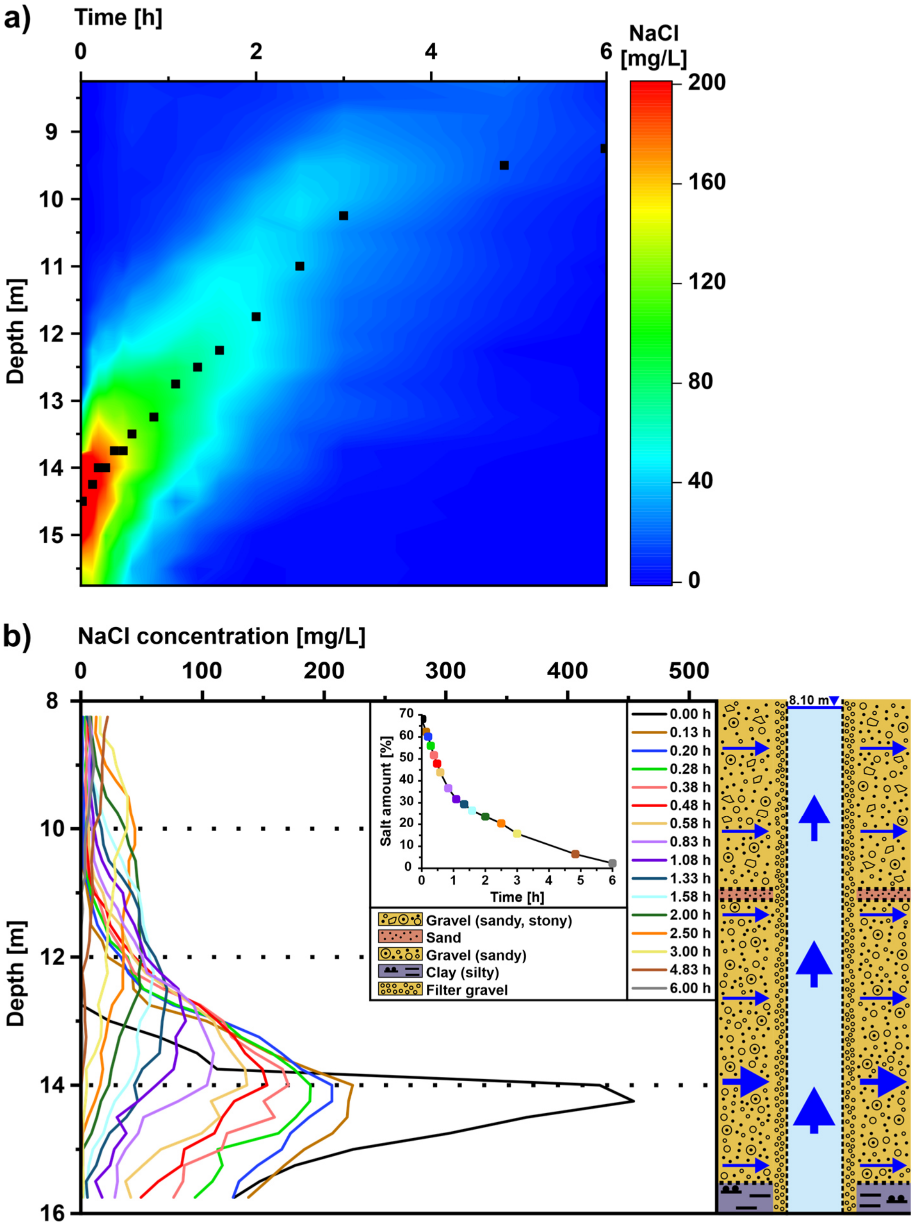

Figure 17: *Point injection in GMW 5312 (18.11.2020); 12.5 g NaCl (500 mL of a 25 g/L solution) were injected at a depth of 14 m.* ***(a)*** *The salt plume shows upward movement within the well, and the black squares indicate the center of the salt plume for each measurement.* ***(b)*** *The fast decrease of salt amount reveals an additional horizontal outflow. The arrows on the right display the groundwater flow within the well derived from the concentration profiles.*

In contrast, ***Figure 18*** shows an example with vertical downward flow from GMW 5303, where 500 mL of a 25 g/L NaCl solution were injected at a depth of 10 m. GMW 5303 shows a rapid downward flow, which already influences the first profile. The following measurements demonstrate the fast vertical flow in the well by the downward movement of the salt plume. The velocity of the downward flow can be estimated at 5.7 m/h based on the mean vertical offset between the measurements.

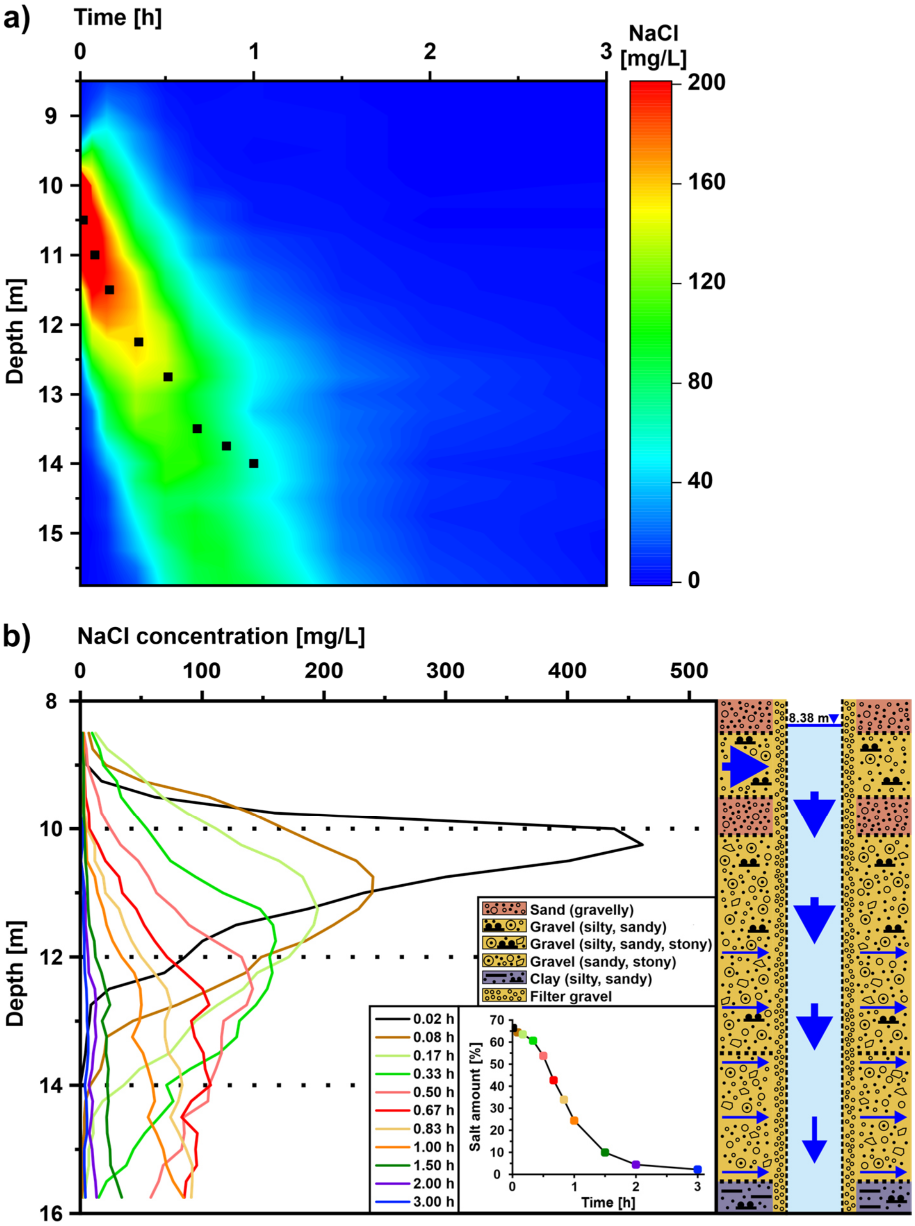

***Figure 18:** Point injection in GMW 5303 (18.11.2020); 12.5 g NaCl (500 mL of a 25 g/L solution) were injected at a depth of 10 m. **(a)** The tracer plume shows a fast downward movement, and **(b)** the salt amount indicates a delayed outflow due to the injection in the upper part of the well and the main outflow in the lower part.*

The development of tracer amount over time shows just a slow decrease in the first 20 minutes. Then, as soon as the tracer plume reaches depths below 12 m, the decrease gets faster, indicating a higher outflow in the lower part of the well. The higher outflow near the bottom can be explained by a higher permeability due to less fine-grained sediments (silt) at this depth. Three other point injections in GMW 5303 in 2018 and 2020 showed similar results. Depending on water level, injection depth and distance to the zone with higher outflow, the half-time (time until 50 % of the trace has left the well) varies between 11 min and 1.5 h.

The third example (***Figure 19***) displays an injection in GMW 7721, which is a karst well with a total depth of 74 m and an already demonstrated vertical flow (Fahrmeier et al. 2021). After the tracer was injected at a depth of 31 m, the salt plume moves downward, and after 9 hours the maximum value is near the bottom of the well. Based on the mean offset, the vertical flow has a velocity of approximately 3.8 m/h.

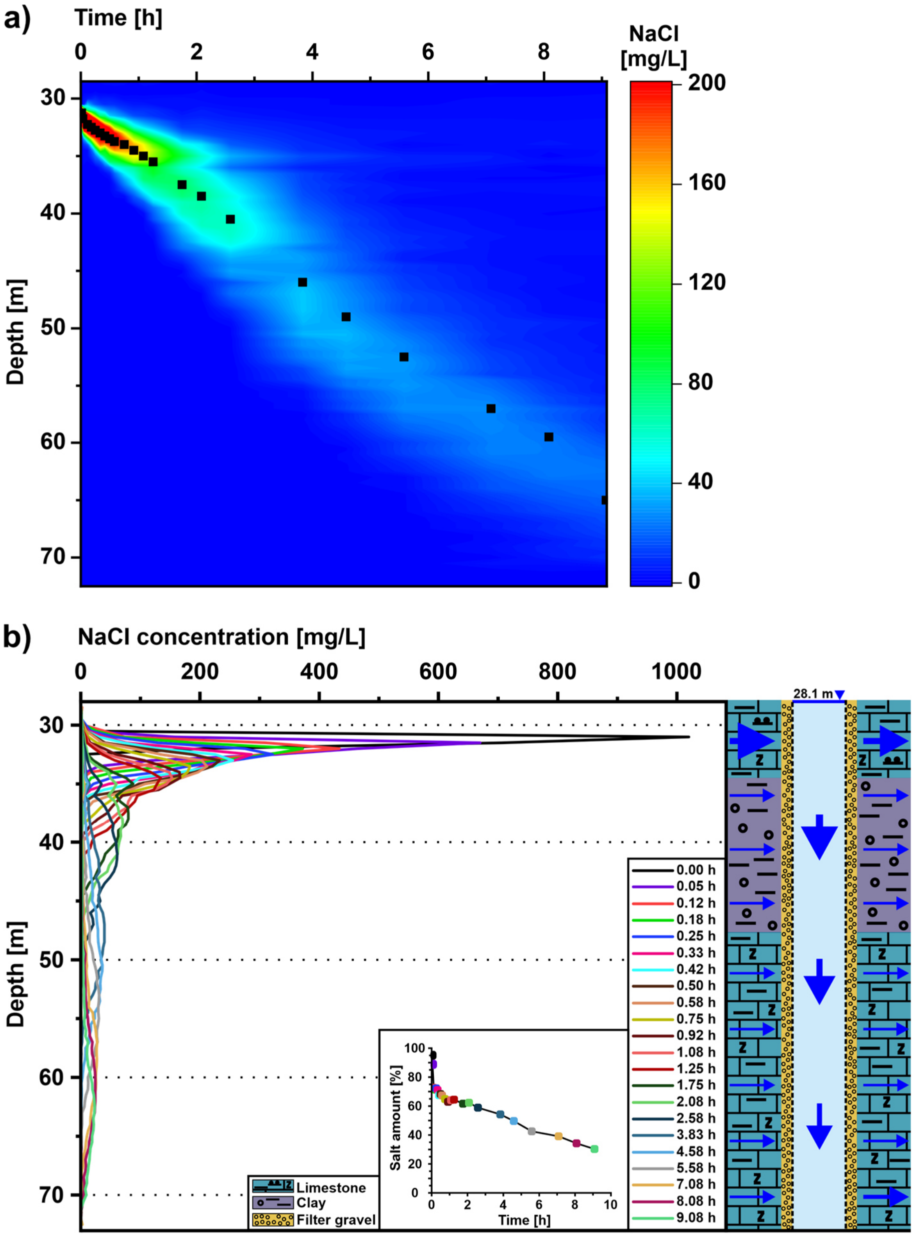

Figure 19: *Point injection in GMW 7721 (17.11.2020). 12.5 g NaCl (500 mL of a 25 g/L solution) were injected at a depth of 31 m.* ***(a)*** *The salt plume moves downward at a steady speed, indicated by the center of the salt plume for each measurement (black squares).* ***(b)*** *A zone with high outflow in the upper part (ca. 30 – 33 m depth) is identifiable through the fast decrease of the salt amount during the first measurements.*

Up to the third measurement, the salt amount shows a strong decrease, which is then decelerated and almost constant. This indicates a strong horizontal flow in the upper part of the well, most likely in the limestone above the clay layer. Below this zone, horizontal flow is less strong but uniform in every depth, since the salt amount shows a continuous decrease. An earlier test with an impeller flowmeter was not able to detect the vertical flow in GMW 7721, since the velocity was too low for the impeller to turn, which is a common problem with these devices (Sellwood et al. 2015). This shows that point injection-SBDTs are better at detecting low velocities. Alternatively, an electromagnetic flowmeter or a heat pulse flowmeter could have been used. The latter, however, is used stationary and would require several measurements to deliver results for an entire well (Sellwood et al. 2015).

3.5 Conclusion

The new probe for point injections in groundwater monitoring wells and boreholes was tested in the laboratory and in the field. The result showed a good reproducibility regarding the shape and extent of the tracer cloud, which proves the suitability of the probe. It is robust and equipped with a well-functioning and reliable opening mechanism. Due to its simplicity, the mechanical mechanism is an advantage compared to existing devices. The probe is easy to handle and can be operated by one person. It is designed to minimize effects on the natural flow within the GMW or aquifer and so it is particularly suitable if vertical flow is relevant and should be observed. Using the new probe, it is not possible to gain absolute velocities for vertical flow, but due to the tracer movement and the shifting of the maximum concentration or the center of the tracer cloud, an approximate value can be estimated. As an advantage over impeller flowmeters, which are not able to detect low vertical velocities, even minimal vertical flow rates can be documented. Compared to other devices and methods, SBTDs with the new point injection probe need less personnel and less equipment; no pumps or electricity is needed, just the probe, tracer (typically NaCl) and a measuring device. This reduces costs and makes the point injection probe suitable for many applications, e.g. study areas with a large number of monitoring wells, and accordingly many necessary tests, but also projects in low-income countries or projects with limited resources. Due to the good portability, it is also practical for testing locations that are difficult to access. Also, the length of the measuring tape is flexible, so the probe can be used in deep wells without depth limitation and without being adapted for each well, which is an advantage compared to existing methods or devices.

With the salt plume extending over 1.75 m for an undisturbed injection profile, it can be considered as a point injection in most wells or boreholes. If the diameter of the tested well or borehole is big enough, preferably the probe remains at the injection depth during the measurements to avoid turbulences that influence the test. If the diameter is smaller than 10 cm, the probe should be carefully lowered to the bottom of the well or borehole before starting the measurements.

If NaCl is used as tracer, low concentrations, e.g. 25 g/L, should be used to avoid or minimize density effects. By the use of uranine or other fluorescence tracers, density effects can be completely avoided, due to the lower concentrations, but a more expensive measuring equipment is required. Diffusional influences are negligible for wells with a good connection to the aquifer, since diffusion is a much slower process compared to groundwater flow. To prevent turbulences induced by the measurements, multiple divers can be preinstalled at fixed depth intervals. Although it does not generate complete profiles, up- or downward movement can be detected this way.

In summary, the new point injection probe is a useful device and a good alternative to the existing methods. Due to the flexibility regarding tracer, aquifer and injection depth, combined with easy handling, it is suitable for the investigation of boreholes and groundwater monitoring wells, which is why a patent has been applied for the probe.

Acknowledgments

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CHAPTER 4

4 Multi-scale characterization of a complex karst and alluvial aquifer system using a combination of different tracer methods

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Abstract

Water suppliers face major challenges such as climate change and population growth. To prepare for the future, a detailed knowledge of water resources is needed. In southern Germany, the state water supply (Zweckverband Landeswasserversorgung) provides 3 million people with drinking water obtained from a complex karst and alluvial aquifer system and the river Danube. In this study a combination of different tracing techniques was used with the goal of a multi-scale characterization of the aquifer system and to gain additional knowledge about groundwater flow toward the extraction wells in the Danube valley.

For the small-scale characterization, selected groundwater monitoring wells were examined using single-borehole dilution tests. With these tests, a wide range of flow behavior could be documented, fast outflow within just a few hours in wells with a good connection to the aquifer, but also durations of multiple weeks in low-permeable formations. Vertical flow, caused by multiple flow horizons or rising groundwater, was detected in 40 % of the tested wells.

A regional multi-tracer test with three injections was used to investigate the aquifer on a large scale. For the highly karstified connections between a swallow hole and a spring group, high flow velocities of around 80 m/h could be documented. Exceptionally delayed arrivals, 250 and 307 days after the injection, showing maximum velocities of 0.44 and 0.39 m/h, were observed in an area where low-permeable sediments overlay the karst conduits.

With the chosen methods a distinct heterogeneity caused by the geological setting could be documented on both scales.

4.1 Introduction

Providing high-quality drinking water is one of the major challenges of increasing severity that every country or region all over the world has to face. These are especially effects of climate change, such as an increasing severity and number of extreme weather events like droughts and heavy rain events, and the increasing population, lead to a growing stress on the global water supply (Bates et al. 2008; Delpla et al. 2009; Hanjra and Qureshi 2010; Wheeler and von Braun 2013; Olmstead 2014; Stevanović 2019). Apart from supplying the population with drinking and process water, a substantial availability of water is also crucial for the prosperity and economic development of a region (Olmstead 2014; World Bank 2016).

In southern Germany, water availability is generally sufficient. However, especially in the beginning of the 20th century, water supply was problematic in some regions, e.g., the Swabian Alb. This historically and culturally important karst landscape (Goldscheider 2019), which is also a UNESCO Global Geopark, is characterized by a distinct karstification of the Jurassic limestones, leading to a lack of surface waters. Also, since the groundwater level is deep below the surface, inhabitants of the Swabian Alb mostly had to rely on dammed ponds with poor quality as water source (Zweckverband Landeswasserversorgung 2012).

Also in the middle Neckar region, water supply has been critical due to problems with water availability and quality, caused by an enormous population increase and fecal contamination. In the course of industrialization, the population in Stuttgart grew from 119,000 to 253,000 between 1882 and 1907 the demand for water could barely be achieved. The development of new water resources was inevitable, especially considering that the region is a center of commerce and industry (Zweckverband Landeswasserversorgung 2012). Ideas to provide Stuttgart with water from Lake Constance, the northern Black Forest, or the Neckar valley were discarded. Finally, the Danube valley was chosen due to its high quality and rich groundwater resources, fed by the inflow from the large Jurassic karst aquifer of the eastern Swabian Alb. Finally, the Zweckverband Landeswasserversorgung (state water supply, LW) was founded in 1912 and the long-distance water supply for Stuttgart and the eastern Swabian Alb was established. Gradually, more cities and communities joined the association, so that today the economically important triangle between Stuttgart, Ulm and Aalen is supplied by the state water supply (Zweckverband Landeswasserversorgung 2012).

Nowadays, high-quality drinking water for approximately 3 million people in Baden-Wuerttemberg is provided with a maximum capacity of 5200 L/s. Most water is gained through more than 200 extraction wells in the Danube valley, with a total maximum extraction rate of 2500 L/s. Additionally, the state water supply extracts water from the Danube, on average 1100 L/s, and the captured Buchbrunnen spring, with up to 800 L/s. For periods of peak demand, deep karst extraction wells near the village Burgberg can be used to provide an extra 500 L/s. In recent years, the average amount of distributed water is around 100 MCM/a (million cubic meters per year, Zweckverband Landeswasserversorgung 2021). Approximately 50 % of this water is obtained from groundwater originating in the karst aquifer, making the state water supply comparable to the largest karst water supplier in Europe, the Vienna water supply, which uses multiple karst springs to provide water for 1.7 million citizens (Stevanović 2019).

Currently, the LW is facing challenges such as climate change, extreme weather events (Haakh 2019), and increasing nitrate concentrations caused by intense agriculture within the groundwater protection area (Haakh 2018). To address and prepare for these tasks, a better knowledge of the catchment area, which extends over the eastern Swabian Alb and parts of the Danube valley, is required. For this reason, a project was launched with the aim of a multi-scale characterization of the complex aquifer system and the flow toward the extraction wells. Due to the distinct heterogeneity of karst, it is very difficult to characterize and represent a karst system in detail with numerical models alone. Here, a combination of tracing techniques on different scales was chosen to identify processes in the catchment, beginning with the western part.

The main objectives of this study were (a) to examine groundwater flow on a small scale by conducting single-borehole dilution tests (SBDT) in groundwater monitoring wells (GMW) focusing on identification of flow horizons, outflow behavior and potential vertical flow, (b) to evaluate selected GMWs with SBDT with regard to their suitability as injection points for a large-scale tracer test, (c) to identify hydraulic connections, flow velocities, and sub-catchments on a regional scale with a multi-tracer test, focusing on groundwater flow from areas with potential contamination risk towards the extraction wells in the Danube valley, and (d) to evaluate the obtained results of the regional tracer tests with regard to the inflow of the extraction wells and their protection concept.

The overall goal of this study is to add to the existing knowledge about the aquifer system and groundwater flow on small- and regional scale, in order to prepare for future challenges.

4.2 Material and Methods

4.2.1 Study site

Groundwater protection area *Donauried-Hürbe*

The groundwater protection area of the state water supply, with more than 510 km² one of the largest in Germany, is located in eastern Baden-Wuerttemberg and was established for the extraction wells in the Danube valley. A total of 204 wells, subdivided into six well fields, extract water either from the Quaternary alluvial aquifer, that is fed by the Jurassic karst aquifer, or directly from the karst aquifer. Each well field has its own pumping station that pumps the extracted water towards the waterworks. The recharge area of the extraction wells is not perfectly represented by the groundwater protection area, since the European watershed (***Figure 20***) crosses the area in the northwest (Schloz et al. 2007). The elevation drops from about 700 m a.s.l. in the area of the watershed to 450 m a.s.l. in the Danube valley.

Geology

From a geological point of view, the water protection area can be divided into two sectors: the Swabian Alb, which is composed of Jurassic limestones and marls, and the alluvial plain of the Danube valley (Donauried), where the limestones are overlain by Oligocene, Miocene, and Quaternary sediments (Schloz et al. 2007).

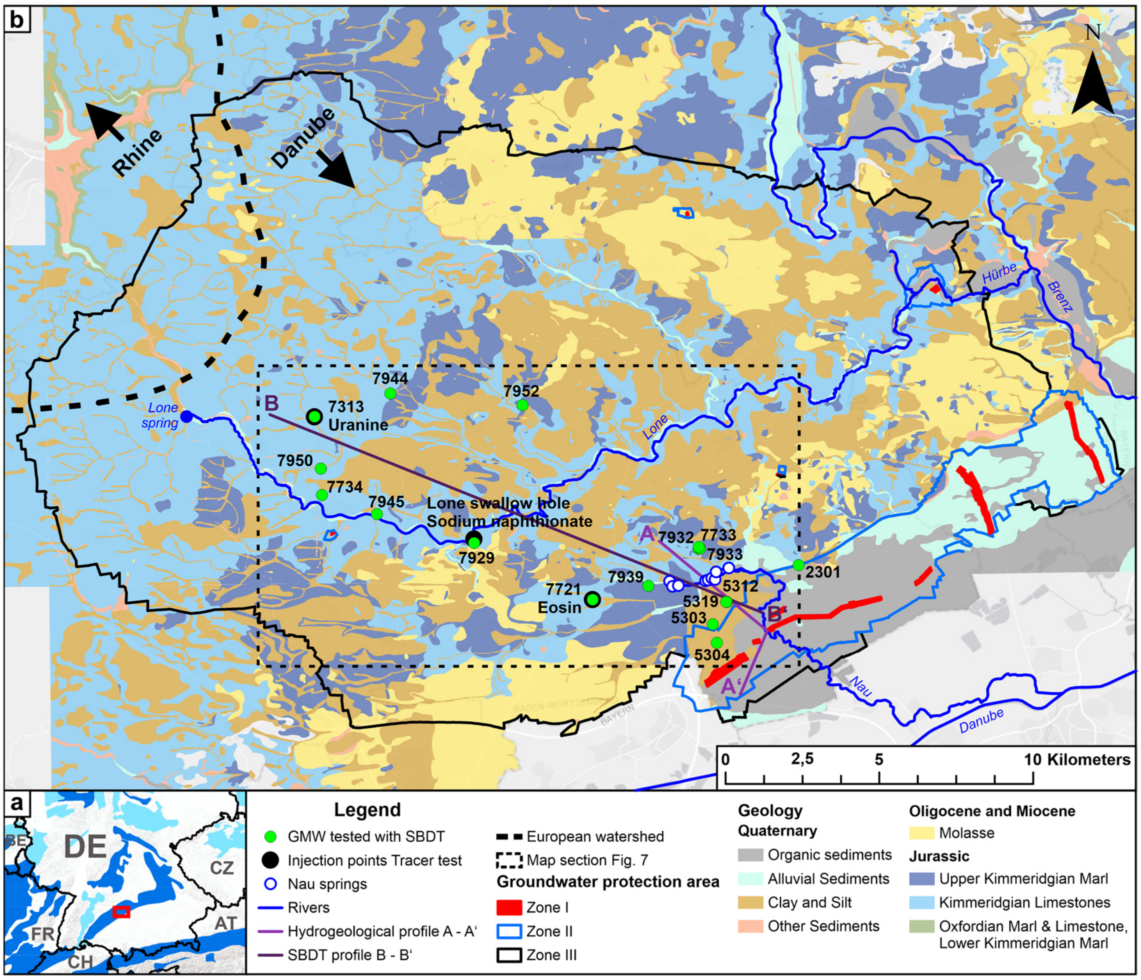

Figure 20: ***(a)*** *Location of the study site (red box) shown on a portion of the World Karst Aquifer Map (WOKAM, Chen et al. 2017. Dark blue: continuous carbonate rocks; light blue: discontinuous carbonate rocks; country codes from International Organization for Standardization 2023).* ***(b)*** *Geological map of the groundwater protection area of the state water supply with locations of groundwater monitoring wells (GMW) tested with single-borehole dilution tests (SBDT).*

The Jurassic formations in the Swabian Alb have thicknesses of up to 400 m and dip gently toward the southeast. In the study area, bedded facies and reef limestones occur, with the latter showing the strongest karstification (Schloz et al. 2007). In the northwestern part of the groundwater monitoring area, Oligocene and Miocene Molasse deposits on top of the limestones are few or entirely absent. Toward the southeast the Molasse covering increases with increasing thickness. In the area of the Danube valley, the limestones are covered almost entirely, with thicknesses up to 90 m (Schloz et al. 2007). In the Danube valley, the Molasse is overlain by Quaternary gravels and sands with thicknesses of up to 11 m. The youngest units are mostly redistributed deposits and river sediments covered by clay, silt, peat or other organic sediments (Udluft et al. 2000; Schloz et al. 2007).

Hydrogeology

The limestones form a large-volume karst aquifer that is underlain by the low-permeability lower Kimmeridgian marls, which form the base of karstification in the catchment (***Figure 21***). The tracer tests in the adjacent areas demonstrate a high degree of heterogeneity with flow velocities of more than 100 m/h, indicating highly karstified zones, mainly toward springs, but low velocities and long travel times in zones with low permeabilities (Kolokotronis et al. 2002). Groundwater recharge is mainly attributed to diffuse percolation of precipitation through shallow soils and epikarst, or small watercourses sinking into swallow holes; the water then flows towards the southeast (Kolokotronis et al. 2002). A large quantity of the karst groundwater transits into the alluvial aquifer, built up by the Quaternary gravels and sands in the Daube valley, in zones where the low-permeable Molasse sediments (k = 10-6 – 10-5 m/s) were eroded, e.g. in the northern part of the Danube valley where the gravels lie directly on top of the Jurassic limestones, or show just minor thicknesses. Additionally, karst groundwater can rise into the alluvial aquifer through fractures in the Molasse (Kolokotronis et al. 2002). Zones with ascending karst groundwater can be localized via temperature anomalies or chemical analyses (Udluft et al. 2000).

In the northwestern part of the groundwater protection area, there is only one large spring, the Lone spring, which discharges 240 L/s on average but up to 3200 L/s during high-flow conditions (Schloz et al. 2007). Based on age dating with tritium, the water of the Lone spring shows an average residence time of 22 years (Kolokotronis et al. 2002). The spring feeds the Lone creek, whose valley crosses the catchment area from west to east. However, due to several swallow holes most of the river bed is dry; water reaches the Hürbe creek only after strong rainfall or during snowmelt. Usually, just the first few kilometers beyond the Lone spring, and the segments beyond the inflow from wastewater treatment plants, are water-bearing.

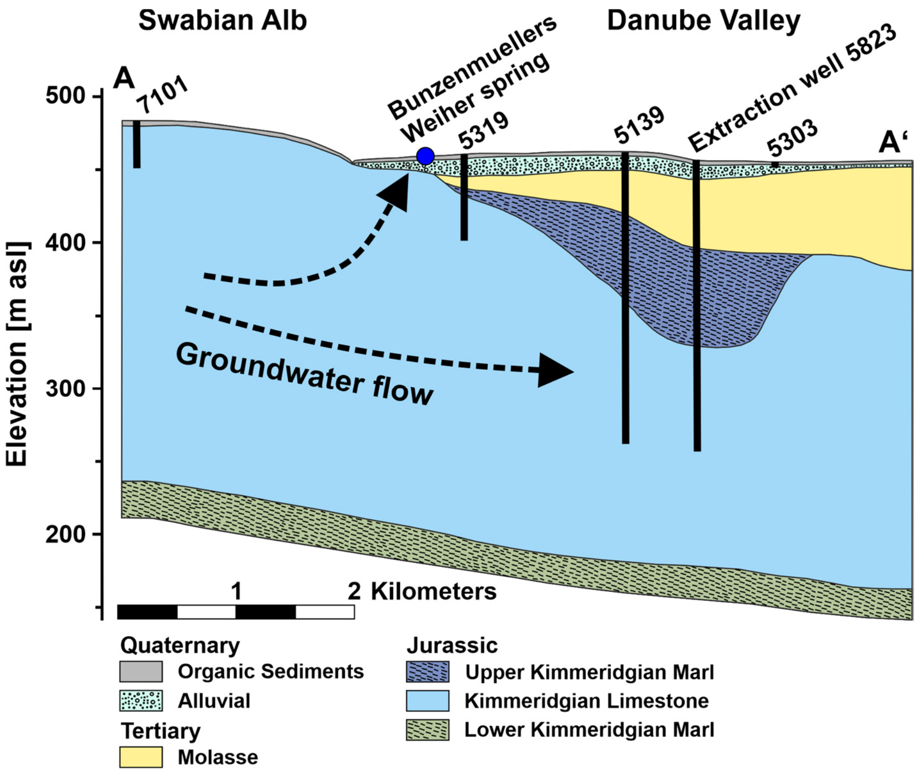

Figure 21: *Hydrogeological profile A – A′. Due to eroded Molasse at the border between Swabian Alb and Danube valley, karst groundwater can flow directly into the alluvial aquifer.*

The Nau springs, the most important springs in the catchment, are located in the town Langenau at the border between the Swabian Alb and Danube valley. A large number of sources, summarized as eight spring groups distributed along the west-east axis through the town, partially discharge the karst groundwater flowing toward the southeast. Discharges of the individual spring groups vary between 5 and more than 200 L/s, the total accounts for an average of 1230 L/s (Schloz et al. 2007). The westernmost spring group, Nauursprung spring, was also dated using tritium, shows a mean residence time of 47 years (Kolokotronis et al. 2002), which, however, does not include any information on the fast-flowing components toward the spring.

In the area surrounding the catchment, numerous tracer tests have been conducted in the past. Yet only one large-scale test with an observed breakthrough was performed in the inflow of the Nau springs and the extraction wells in the Danube valley. 25 kg of uranine were injected in an active swallow hole southwest of Gerstetten on 02.12.1969 and detected at Nauursprung Spring. After Kolokotronis et al. (2002) two values for the maximum velocity can be found, 352 and 823 m/h. Since comparable tests in the surrounding area show maxima between 23 and 167 m/h, Kolokotronis et al. (2002) assess the obtained velocities as questionable.

4.2.2 Single-Borehole Dilution Test methods

SBDTs are based on the injection of tracer, e.g. fluorescence dyes, NaCl, or heated water, in the saturated zone of a borehole or well, followed by the observation of outflow with measurements of multiple concentration profiles (Brouyère et al. 2008; Maurice et al. 2011; Banks et al. 2014; Libby and Robbins 2014; Read et al. 2014; Poulsen et al. 2019b; Fahrmeier et al. 2021). SBDTs can be conducted as uniform injections over the entire saturated length, delivering results for the whole well or borehole. For detailed information of one specific depth or the investigation of vertical flow, point injections can be used (Maurice et al. 2011).

Most uniform injections were performed using fine-grained NaCl and a Permeable Injection Bag (PIB) to achieve a homogeneous tracer concentration in the well (Fahrmeier et al. 2021). Others were conducted using the hosepipe method, which involves lowering a hosepipe into the well, filling it with tracer solution, and then pulling it out with a constant speed to obtain a uniform injection (West and Odling 2007; Maurice et al. 2011). Point injections were conducted with a newly developed injection probe, that contains tracer solution and is opened by dropping a weight down the line (Fahrmeier et al. 2022). After all injections, multiple profiles of the electrical conductivity were measured in time intervals that were chosen depending on the recorded changes. The method by which the data were further analyzed is described in Fahrmeier et al. (2021).

Between 2016 and 2021, 17 different GMWs in the groundwater protection area were tested using SBDTs. 13 of them are karst GMWs covering depth ranges between 9 and 122 m, with the longest saturated length being 51 m. The other four are alluvial GMWs located in the Danube valley with depths up to 16 m. A total of 51 SBDTs were conducted, 41 of which were uniform injections (28 in karst wells, 13 in alluvial wells), mostly conducted with the PIB-method. The other 10 were point injections in karst wells (3) and alluvial wells (7).

Goals of the SBDTs were, to identify possible injection points for the regional tracer, groundwater flow through and within monitoring wells, evaluate the connection to the aquifer, and detect in- and outflow horizons, as well as vertical flow. Also, with results from multiple wells, an overall hydraulic characterization of the aquifer and its flow conditions was the objective.

4.2.3 Regional multi-tracer test

Within the scope of this study, possible tracer injection points, swallow holes and GMWs, were identified within the catchment area. To test the GMWs connection to the aquifer, uniform SBDTs were conducted in selected wells. Besides the flow conditions, the proximity to areas or industry with an increased contamination risk was taken into account. For the multi-tracer test, three injection points representing the western inflow were chosen (***Figure 20***).

16 kg of uranine were injected in GMW 7313 on 11.10.2017. This site was chosen due to its large distance to the extraction wells, with the goal to characterize flow from distant parts of the catchment area. Two SBDTs conducted in the well before the tracer test showed an outflow zone from the water level, between 60 and 65 m, to a depth of 70 m (all depths refer to the respective

well cap); below this zone the well showed just minor outflow. To cut off the inactive part of the well, a hydraulic packer was installed in a depth of 70 m before injecting the uranine using a hosepipe. After removing the packer two weeks later, a measurement of a concentration profile with a borehole field fluorometer showed only minimal uranine concentrations below 70 m, indicating that the packer functioned.

Also on the 11.10.2017, 95 kg of sodium naphthionate were injected in the Lone swallow hole north of the village Bernstadt. Just 500 m upstream of the swallow hole, a wastewater treatment plant discharges its water into the Lone, which poses a potential risk. In the event of a technical problem in the treatment process, contaminants can be transported into the aquifer within less than one hour. Due to several beaver dams, the swallow hole was not active, but in accordance with the local authorities we were allowed to open the dams slightly, resulting in a steady infiltration for several hours.

14 kg of eosin were injected in GMW 7721 on 12.10.2017. This particular GMW was chosen due to its location close to a hazardous materials storage and an old landfill site. Also, with a saturated length of approximately 50 m, it covers a large depth range and shows a fast outflow over the entire length. For this reason, the tracer was distributed throughout the well by moving the hosepipe up and down during the injection.

A total of 72 sampling points, including springs, surface water, pumping stations, extraction wells, alluvial and karst-GMWs, were monitored using water samples, manual and automated, activated charcoal adapters and field fluorometers. Especially due to the sodium naphthionate injection into a natural swallow hole, the sampling was designed to cover potential fast flow velocities towards the Nau springs and in particular the westernmost Nauursprung spring, where one of the fluorometers was placed. The other was installed to monitor a deep artesian karst well that is used by the state water supply. The sampling is still ongoing, but the intervals were adapted several times since the injections. Water samples, as well as the activated charcoal adapters, are analyzed in the laboratory using a fluorescence spectrometer LS-55 from PerkinElmer (Waltham, USA).

With linear distances between injection points and the extraction wells in the Danube valley of up to 18.5 km, the regional multi-tracer test covers a very large scale. Tracer tests spanning comparable distances were realized by Kogovšek and Petrič (2004), Petrič et al. (2018) and Fronzi et al. (2020).

4.3 Results and Discussion

4.3.1 Results of Single-Borehole Dilution Tests

With the SBDTs a wide range of different flow behaviors and outflow times could be documented for the GMWs in the protection area. In ***Figure 22***, three examples of SBDT-results from karst-

GMWs are displayed. ***Figure 22 a*** shows the results of a point injection in GMW 7950, where a previous uniform injection indicated a good connection to the aquifer and fast outflow. Assumed vertical flow was verified with the point injection showing a clear upward movement of the tracer plume. Based on both tests, an inflow in a depth of 63 m and an outflow at around 39 m were identified. Since the decrease of salt amount during the point injection is negligible until the plume reaches the top (approx. 0.6 h), no other significant outflows are present in between. The SBDTs in GMW 7950 showed that already in the higher parts of the catchment, multiple conduit levels with different hydraulic head exist. In this case, the higher hydraulic head in the deeper flow horizon results in upward flow within the well.

Figure 22 b shows normalized concentration profiles of a uniform injection-SBDT in GMW 7945. Based on the fast decrease of NaCl concentration, the major flow horizon was identified in a depth of 36 m. After 5.25 h, the remaining salt amount is around 23 % of the injected mass, indicating that the well overall shows a good connection to the aquifer. Slower outflow in the lower part is indicated by remaining NaCl concentrations 20 h after the injection. GMW 7929 (***Figure 22 c***) is located close to the sodium naphthionate injection point. With a uniform injection, the fastest decrease was identified in a depth of 20 m. Compared to the other two wells, the overall outflow is significantly slower. Two days after the injection, concentrations in the upper part almost reached the background, however, in the lower part still around 40 % of the initial concentrations were measured.

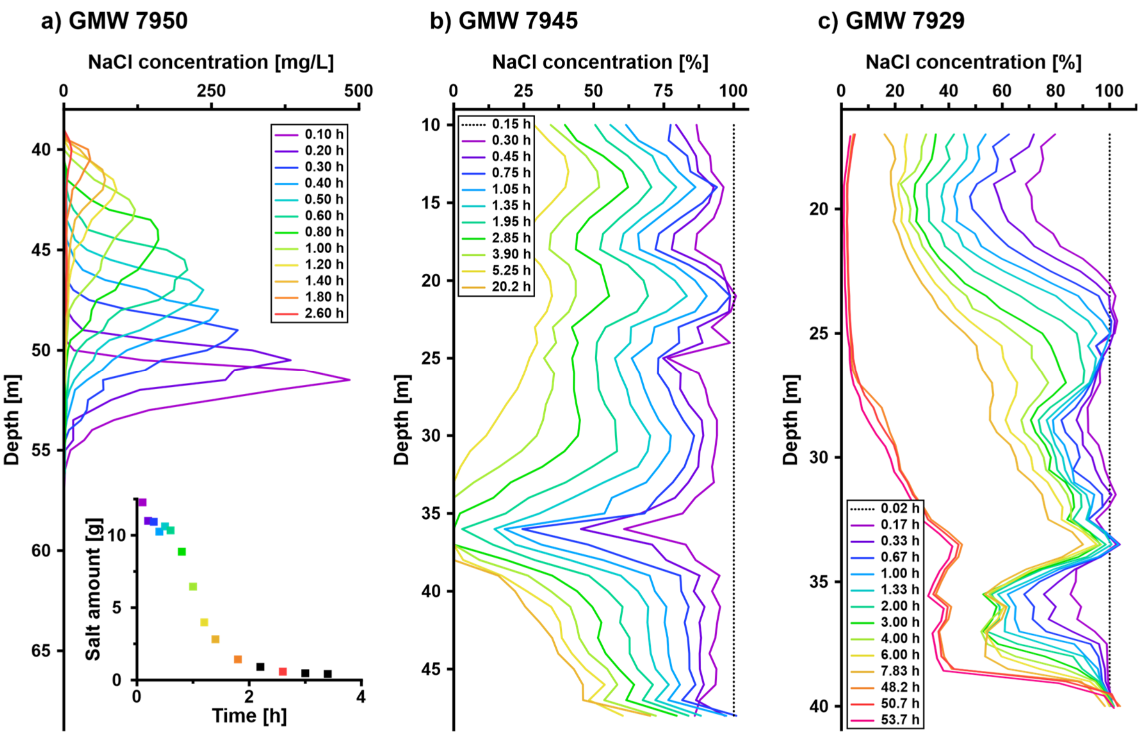

Figure 22: (a) *Results of the point injection in GMW 7950 on 20.04.2021 showing a fast upward movement of the tracer plume.* ***(b)*** *Normalized concentration profiles of a uniform injection in GMW 7945, with the major flow horizon in a depth of 36 m.* ***(c)*** *Normalized concentration profiles of a uniform injection in GMW 7929, which shows a significantly slower outflow.*

With all SBDTs a broad range of behaviors could be documented for the wells in the western part of the catchment. Half-times, the time when 50 % of the tracer has flowed out of the respective well, vary between ten minutes and 22 days. The longest test was monitored for more than 34 days. While the alluvial wells generally showed a faster outflow than the karst wells, some of the latter, e.g. GMW 7733 or GMW 7721, also showed an extremely good connection to the aquifer and a fast decrease of tracer amount.

40 % of the tested wells showed vertical flow (***Figure 23***), which was mostly expected in the karst aquifer, but out of the 13 karst GMWs only two showed an upward movement and only one downward flow. In the upper part of the catchment, the main recharge area, downward movement as part of the regional flow system was assumed. However, with the upward movement in GMW 7950 only the existence of multiple conduit levels could be documented. GMW 7721, showed a combination of vertical and horizontal flow, which fits the regional model, but might also be induced by local conditions, e.g. a stream that infiltrates into the aquifer close to the well. The upward flow in GMW 7932 suggests that karst groundwater rises in the area before the karst aquifer is overlain by the low-permeable Molasse and flows towards the Nau springs or directly into the alluvial aquifer.

With regard to the alluvium, usually no distinct vertical flow would be assumed in a shallow and homogenous alluvial aquifer. However, due to the special hydrogeological setting in the groundwater protection area, with karst groundwater ascending into the alluvial aquifer, vertical flow was documented in all tested alluvial GMWs. Consequently, the two wells with upward movement are most likely located in areas with uprising karst groundwater while downward flow in the other wells is induced by compensatory movement.

Depth-dependent outflow differences were documented in multiple wells, e.g. GMW 7313, which shows a good connection in the upper part, but in the lower part, increased NaCl concentrations were still measured 34 days after the injection. Also, wells close to each other showed a different behavior. GMWs 7733, 7932 and 7933 form a triangle with side lengths between 50 and 60 m. Despite these small distances, each well shows a different flow behavior. GMW 7733 is well-connected to the aquifer with the major flow horizon in a depth of 29 m and no vertical flow. GMW 7932 has approximately the same outflow horizon, but also an inflow near the bottom and a resulting vertical upward movement. GMW 7933 is poorly connected to the aquifer and shows no vertical flow component. Regarding both depth and distance, these distinct differences can be explained by the characteristic heterogeneity of karst aquifers that, in this case, could be nicely documented on a small scale, using borehole dilution tests.

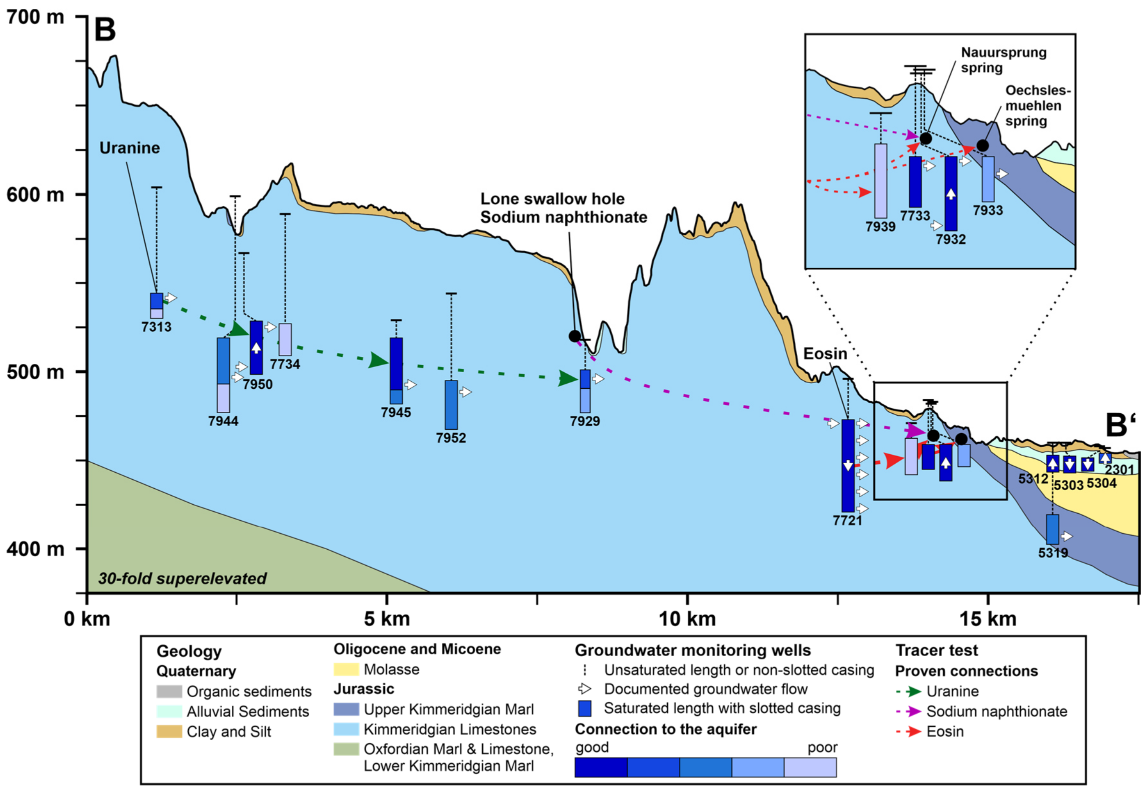

Figure 23: *Graphical overview of all SBDT-results and detected connections during the tracer test. All GMWs were projected on profile B – B′ (**Figure 20**) parallel to the strike of the Jurassic limestones.*

4.3.2 Regional multi-tracer test

With the selected monitoring network all three injected tracers could be detected. While sodium naphthionate and eosin arrived at the Nau springs, uranine concentrations were measured in three karst GMWs southeast of the injection well. However, no tracer has been observed in the extraction wells so far.

90 h after the injection, sodium naphthionate was detected in a water sample from monitoring point NU1, which covers the hole group of sources at Nauursprung spring. With the high-resolution data of the field fluorometer the first arrival cold be determined at around 80 h (***Table* 5*)***. 114.5 h after the injection, sodium naphthionate was also detected at NU2, an additional sampling point upstream of NU1. This leads to the conclusion that multiple sources must exist in the area of the Nauursprung spring which can also be seen based on the breakthrough curves (BTC; ***Figure 24***). While a high conformity of water samples and field fluorometer data is given, the latter shows three peaks. While the first one, around 100 h after the injection, represents the first arrival at the spring group, the second peak, after ca. 115 h, can be explained through the high concentrations arriving at NU2. Due to the larger interval this behavior is not visible in the water sample data. The same applies for the third peak after approximately 135 h.

Table 5: *Descriptive parameters of the sodium naphthionate breakthrough at Nauursprung spring (WS = water samples; FF = field fluorometer).*

	NU1 WS	NU1 FF	NU2 WS
Distance [m]	6630	6630	6500
First detection [h]	90.4	ca. 80	114.5
V_{max} [m/h]	73.3	ca. 82.5	56.8
V_{dom} [m/h]	66.9	69.4	56.8
C_{max} [µg/L]	2.54	3.06	5.01
Recovery [%]	ca. 0.03	ca. 0.03	-

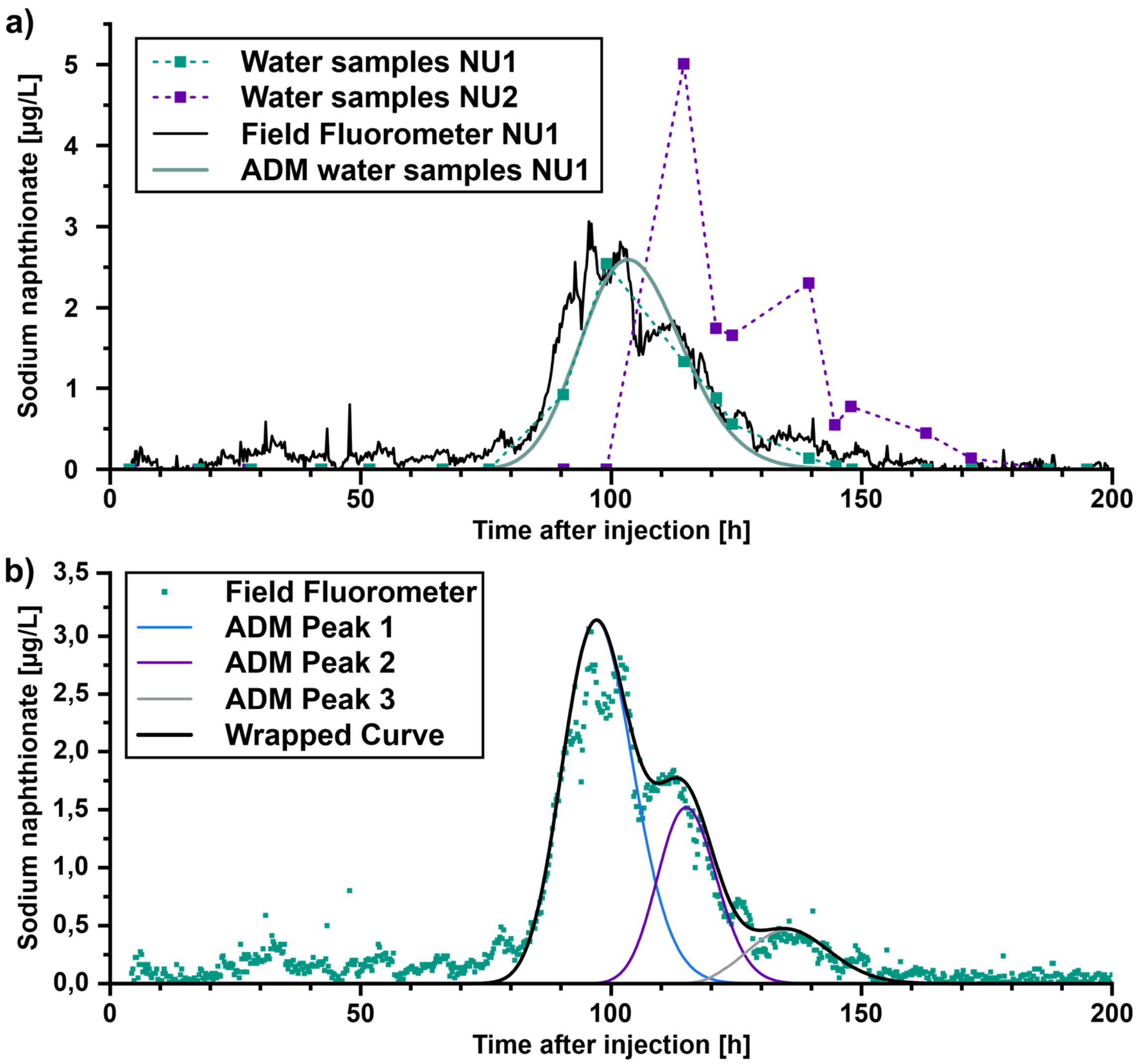

Figure 24: ***(a)*** *Sodium naphthionate breakthrough curves (BTC) at Nauursprung spring monitored with water samples and a field fluorometer. While NU2 is a sampling point close to one of the sources, NU1 is further downstream and covers the whole spring group.* ***(b)*** *shows the field fluorometer data with the fitted ADM (Advection-Dispersion Model) curves for the three identified peaks and the wrapped curve.*

For Nauursprung spring, a recovery rate of around 0.03 % was calculated. Since no further sodium naphthionate concentrations were detected, additional flow paths have to exist, leading towards deeper layers of the aquifer with long residence times. This explains that no other sampling point showed sodium naphthionate concentrations. Also, due to the enormous groundwater volume in the aquifer system, dilution can occur to an extent below the limit of detection.

Regarding the eosin, a transport towards the Southeast and especially to the deep artesian karst wells was expected on the basis of groundwater contour lines. However, after three days, eosin was detected in GMW 7939, which is poorly connected to the aquifer, as shown by a SBDT (***Figure 23***) and geophysical borehole logging, and located east-northeast of the injection point. 250 days after the injection, the tracer arrived at Nauursprung spring (NU1) and after 307 days at Öchslesmühlen spring (OMS), both of which are located in a similar direction. The descriptive parameters obtained from the BTCs measured at the two springs and GMW 7939 are summarized in ***Table 6***.

Table 6: *Descriptive parameters of the eosin breakthrough at Nauursprung spring (NU1) and Öchslesmühlen spring (OMS).*

	GMW 7939	NU1	OMS
Distance [m]	1870	2640	2850
First detection [d]	3	250	307
V_{max} [m/h]	26.12	0.44	0.39
V_{dom} [m/h]	26.12	0.19	0.21
C_{max} [µg/L]	0.50	0.19	0.12
Recovery* [%]	-	ca. 5.1	ca. 2.4

* Until December 2021

The time gap between the detection in the GMW and the springs can be explained by the geological setting in this area. Following the injection, eosin was transported towards the springs through a karst conduit which is blocked by low-permeable sediments, either Molasse or Quaternary clays and silt, before the springs. This leads to an infiltration of eosin into the limestone matrix and also into GMW 7939. As the second effect of the low-permeable sediments, the further transport towards the springs is decelerated, explaining the exceptionally long travel times until the first detection and the still ongoing breakthrough.

The eosin BTC documented at NU1 and OMS are characterized by low and strongly fluctuating concentrations (***Figure 25***) and are a result of the specific setting. Nauursprung spring covers a large catchment with different flow times, as proven with the fast arrival of sodium naphthionate; a similar situation can be assumed for the nearby OMS. This leads to varying discharge conditions and variable dilution before the tracer reaches the sampling points. A heterogenic catchment also explains, why a correlation between precipitation and tracer concentrations is not possible.

Additionally, minor tracer degradation via ultraviolet radiation can contribute to the fluctuations, since the eosin is exposed to sunlight between the direct sources and the sampling points. However, due to changing flow conditions and weather, this effect cannot be quantified.

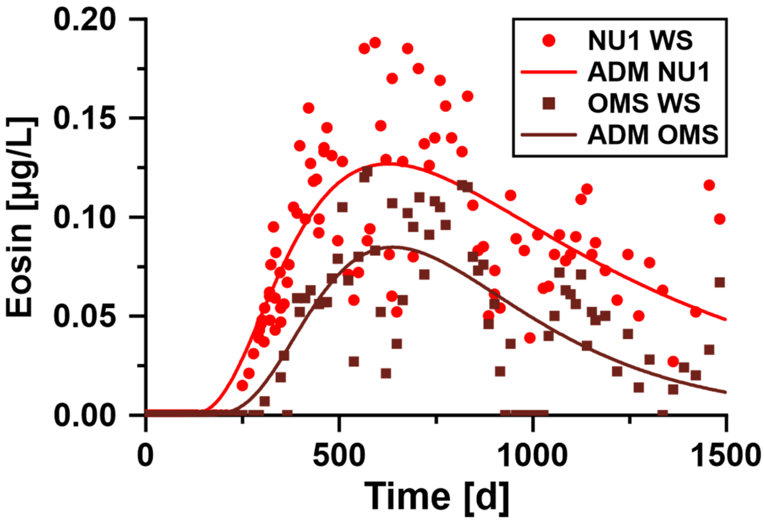

Figure 25: *Eosin concentrations obtained from water samples at Nauursprung spring and OMS with the respective fitted ADM curve.*

Uranine concentrations were detected in GMWs 7950, 7945 and 7929, all of them located in the expected flow direction, 62 days after the injection (***Table*** *7*). During the following sampling, only GMW 7945 still showed marginal uranine concentrations. Since the dilution tests showed fast groundwater flow, especially for GMWs 7950 and 7945, it is possible that they are connected to the conduit system that transports the uranine towards the southeast. The delayed detections are most likely due to low flow velocities between the injection well and the karst conduit, but then fast transport within the conduit system.

Table *7: Summary of the uranine detections in three karst GMWs.*

	GMW 7950	GMW 7945	GMW 7929
Distance [m]	1700	3760	6590
First detection [h]	1487.7	1488.2	1488.5
V_{max} [m/h]	1.14	2.53	4.43
C_{max} [µg/L]	0.23	0.06	0.27

A future detection of uranine at the springs or in the extraction wells cannot yet be ruled out. The long distance in combination with the possibility of low-permeable sediments blocking the conduits could lead to an extremely delayed arrival at the springs or wells. In addition, low-flow conditions were predominant since the injections, resulting in very low hydraulic gradients. All results of the multi-tracer test until December 2021 are summarized in ***Figure 26***.

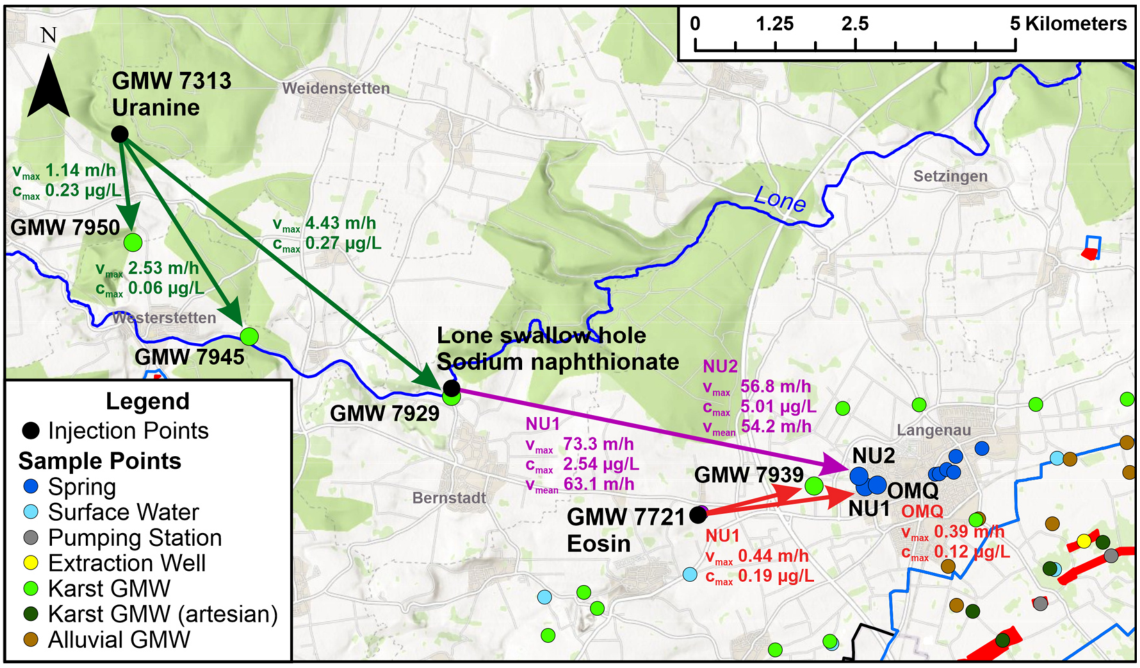

Figure 26: *Results of the regional multi-tracer test four years after the injections.*

The breakthrough curves documented at NU1 and OMS were modeled to obtain transport parameters. Due to the fluctuating concentrations, especially of the eosin breakthrough, a robust approach based on the Advection-Dispersion equation (Kreft and Zuber 1978) was chosen; the modeled curves are shown in ***Figure 24*** and ***Figure 25***, the parameters in ***Table 8***.

Table 8: *Summary of the modeled transport parameters for the BTC of Sodium naphthionate and eosin.*

	Sodium naphthionate				Eosin	
	NU1	FF Peak 1	FF Peak 2	FF Peak 3	NU1	OMS
Mean velocity [m/h]	63.2	67.8	57.4	45.8	0.10	0.14
Dispersion [m²/h]	1970	1165	492	587	54	38
Longitudinal Dispersivity [m]	31.2	17.2	8.6	12.0	552.6	265.9
PD-value [-]	0.0047	0.0026	0.0013	0.0018	0.2093	0.0933
Peclet-number [-]	212.7	385.8	773.4	550.2	4.8	10.7
R^2	0.9859	0.9620	0.9620	0.9620	0.8225	0.7178

For sodium naphthionate the modeling resulted in characteristic longitudinal dispersions for limestones of the Swabian Alb: 1970 m²/h for the water samples and between 492 and 1165 m²/h for the different peaks of the field fluorometer. The eosin values until December 2021, 54 m²/h for NU1 and 38 m²/h for OMS, are amongst the lowest recorded in this formation, the same applies for the documented flow velocities (***Figure 27***). Regarding the relation of distance and dispersivity (***Figure 28***), all calculated values are within the expectable order of magnitude, only the dispersivity of the sodium naphthionate breakthroughs are a little below average.

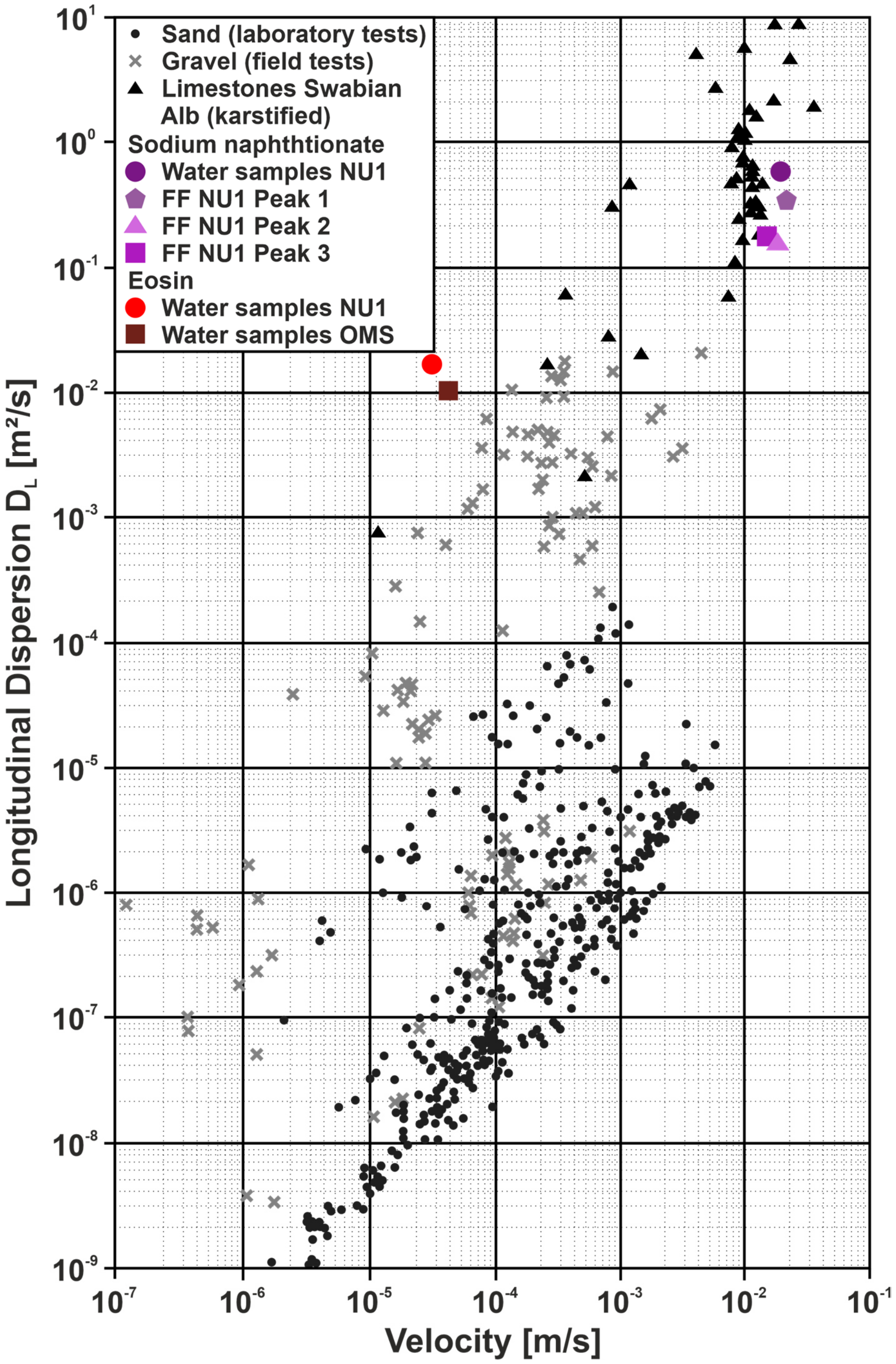

Figure 27: *Relation of Dispersion and Velocity obtained from laboratory and field tests (modified after Strayle et al. 1994). While the sodium naphthionate breakthrough shows typical values for limestones of the Swabian Alb, both eosin breakthroughs show almost the lowest documented velocities and dispersions.*

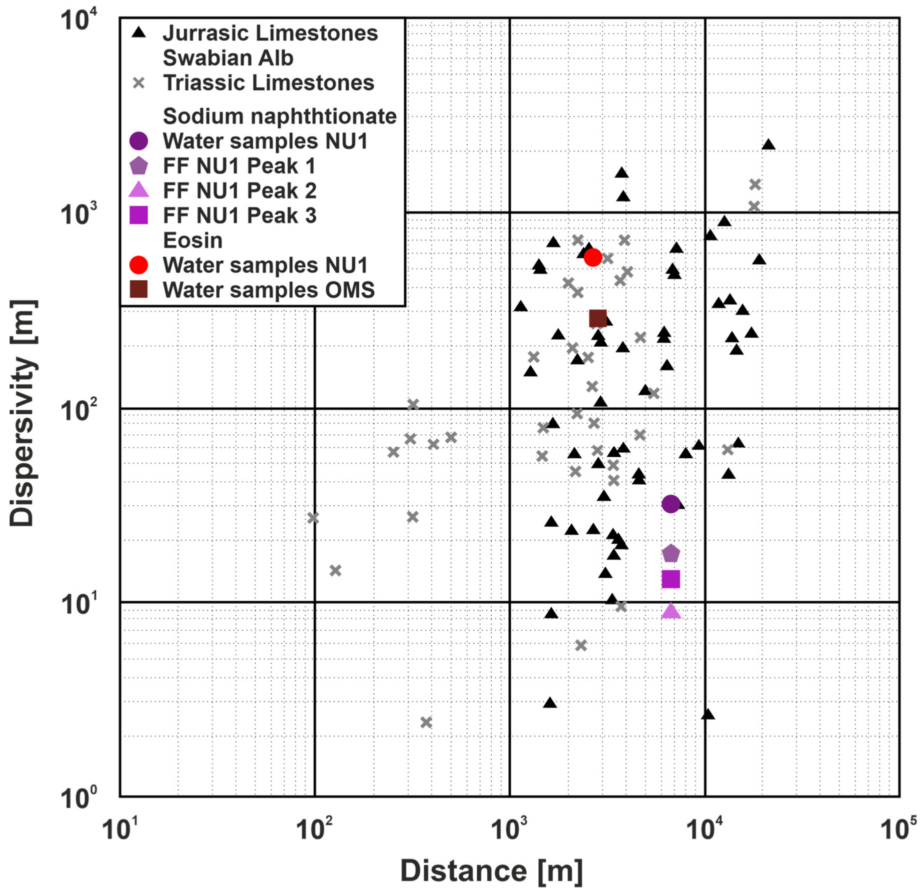

Figure 28: *Relation of Distance and Dispersivity for Jurassic and Triassic limestones (modified after Strayle et al. 1994). The values determined from the breakthroughs at Nauursprung spring and OMS fit well to the existing data.*

The large-scale tracer test conducted within the scope of this project covered large distances, up to 18.5 km between injection and the extraction wells in the Danube valley, and showed exceptional long travel times. Comparable results were observed in the artesian karst aquifer below Stuttgart and in the Unica catchment in Slovenia, both showing breakthrough durations of more than 500 days (Goldscheider et al. 2003; Goldscheider 2008; Kogovšek and Petrič 2014; Petrič et al. 2018).

With the breakthroughs at Nauursprung spring two different behaviors could be observed. The fast arrival and the high flow velocities resulted from the sodium naphthionate injection confirms a well-developed karst conduit which must open directly into the pond. Despite a lower distance, the eosin arrived significantly later due to low-permeable sediments blocking the conduits, resulting in a more diffuse transport towards the springs. A schematic illustration of this setting is shown in ***Figure 29***.

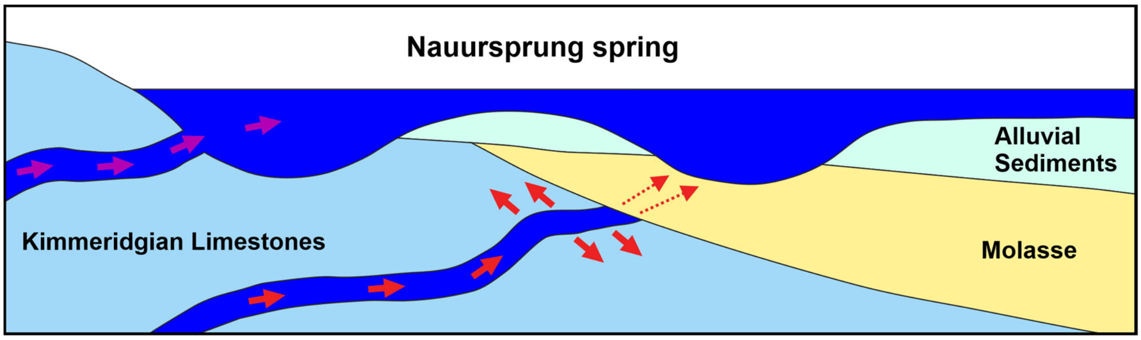

Figure 29: *Schematic interpretation of the two different behaviors documented at Nauursprung spring. The conduit transporting the sodium naphthionate opens directly into the pond, allowing fast flow and transport of dissolved substances. Other conduits are blocked by low-permeable sediments, leading to low flow velocities and a delayed arrival of eosin at the spring.*

4.4 Conclusions

Within this study a complex karst and alluvial aquifer system with supraregional importance for water supply was characterized using a combination of different tracing techniques. For small-scale results, a total of 51 single-borehole dilution tests were performed in 17 groundwater monitoring wells. A regional multi-tracer test was conducted to investigate groundwater flow on a larger scale.

The main conclusions are:

- The tested groundwater monitoring wells showed a wide range of results regarding connection to the aquifer and outflow behavior. Vertical flow was detected in 40 % of the wells, partially caused by uprising karst groundwater in the Danube valley. The duration of tracer outflow varied from a few hours for wells with a good connection to the aquifer and active flow horizons to more than 34 days for wells in low-permeable formations. Also, depth-dependent differences within single wells were documented.
- Several groundwater monitoring wells with a good connection to the aquifer were identified as possible injection points for large-scale tracer tests using borehole dilution tests.
- With the large-scale tracer test, variable flow systems and different hydraulic connections were documented in the study area. High karstification between a swallow hole and Nauursprung spring lead to a fast tracer breakthrough with maximum velocities of around 80 m/h. In contrast, due to low-permeable sediments, another connection to the same spring showed an exceptional delayed arrival, with a first detection after 250 days and a maximum velocity of 0.44 m/h.
- Despite the high extraction rates, no tracer concentrations were detected in the extraction wells in the Danube valley. This confirms long residence times and also the effectiveness

of the existing protection concept. However, the hydraulic situation and the low-flow conditions must be considered for all results.

Overall, the chosen methods have proven to be applicable for an examination of a complex aquifer system. In the groundwater protection area Donauried-Hürbe, a distinct heterogeneity caused by the geological setting could be documented.

Since eosin concentrations are still being measured at the springs, more than four years after the injection, the sampling for the multi-tracer test is still ongoing, to document the breakthrough completely and also to maybe detect tracer in the extraction wells. To complement the results of the western part, the project will be continued in the eastern part of the groundwater protection area with several SBDTs and a second multi-tracer test with shorter distances to the extraction wells in the Danube valley.

Acknowledgments

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CHAPTER 5

5 Synthesis

5.1 Summary and conclusion

5.1.1 Single-borehole dilution test methods

In the first two studies (***Chapter 2***, ***Chapter 3***) this thesis addresses different injection methods for single-borehole dilution tests (SBDTs) under natural conditions. In the first study (***Chapter 2***) a simplified uniform injection method is presented that is suitable to investigate hydraulic processes throughout the whole saturated length of a borehole or groundwater monitoring well. The new method is advantageous compared to existing methods, since it works with commonly available materials at low expense and is flexible in terms of well depths and saturated lengths.

The developed method uses a bag out of nylon mesh filled with sodium chloride (NaCl), which is attached to a rope or a measuring tape and moved up and down in the saturated zone to dissolve the salt and to achieve a uniform distribution within the well. This simplified permeable injection bag method (PIB) is evaluated and compared to the widely used hosepipe method. Several tests are conducted with both methods in the laboratory as well as in groundwater monitoring wells at the study site on the Swabian Alb. Even though the field tests are carried out in wells equipped with slotted casing, both methods deliver meaningful results and detect all major flowing features as well as the heterogeneity of groundwater flow. In some cases, injections with the PIB method produce uneven injection profiles, however, in wells without vertical flow this can be compensated by normalizing the concentrations to the first measurement.

Furthermore, for tests with both injection methods apparent filtration velocities are calculated using linear regression as well as CXTFIT. Both computation methods deliver similar velocities for repeated tests. If the permeabilities of the formation surrounding a well are known, the correction factor α (Equation 10) can be used to calculate the actual filtration velocities. However, the calculation of flow velocities is only valid if no vertical flow components are present that influence the test results.

The results of the first study are that the PIB-method is a well-functioning alternative to the existing methods for uniform injections and allows also allows for the calculation of horizontal filtration velocities. Major advantages of the simplified PIB method are its simplicity and flexibility regarding depth or diameter of the well. It can be used in all types of wells or boreholes without needing to change the equipment and is therefore especially suitable for areas with a large number of wells with varying depths. Also, it is cost efficient, very easy to conduct, even by a single person, and still produces meaningful and valuable results for all aquifer types. With these findings, the PIB method answers the first three research questions positively.

The second study (***Chapter 3***) addresses point injection-SBDTs, which are usually conducted to complement the results of uniform injection-SBDTs. Tracer injections in a discrete depth interval and not throughout the whole saturated length are mostly used to investigate specific depth intervals in deep wells and vertical flow. The latter is especially interesting in karst and fractured aquifers, where vertical flow is frequent due to varying pressures in different conduit or fracture systems that can be intersected by groundwater monitoring wells. Many common SBDT methods do not deliver results on natural vertical flow, either due to the use of pumps or because of hydraulic packers that cut off any vertical flow components. However, information on natural vertical flow can be important for the characterization and understanding of aquifer systems, underlining the importance of natural gradient point injection methods.

This study introduces a device that can be used to inject tracer only into a targeted depth interval of a well or borehole without influencing natural groundwater flow within the well. Moreover, it is easy to handle and equipped with a simple but reliable mechanical opening mechanism. The prototype was built in cooperation with a precision engineer and optimized based on first laboratory test results.

The developed injection probe consists of a container that is attached to a measuring tape and can be filled with a solution of the preferred tracer, lowered into the well and opened by dropping a falling weight down along the measuring tape. When the weight hits the probe, the opening mechanism is triggered and the outer part of the container sinks down, releasing the tracer into the surrounding groundwater.

The probe is evaluated based on several tests conducted in an acrylic glass tube in the laboratory and groundwater monitoring wells in the study site on the Swabian Alb that are known to have vertical flow. The results show that the tracer plume after an injection just extends to 1.5 or 1.75 m, which can be considered as a point injection, especially in deep wells that are likely to have a vertical flow component. According to the laboratory tests, the probe is able to reproduce similar tracer plumes for repeated injections. Knowing the undisturbed shape of the tracer plume facilitated the interpretation of the field tests, since the first measurements after the respective injections are already influenced by the natural vertical flow within the wells.

With its simple but reliable mechanical mechanism and low productions costs, in combination with the good results in the field tests as well as the proven reproducibility of the injection profile, the probe is a progress compared to existing methods and successfully addresses the research questions 4 – 6. Due to the many possible applications of the injection probe, the decision was made to apply for a patent. The application is currently examined by the patent office.

5.1.2 Multi-scale characterization of the groundwater protection area

The third study (***Chapter 4***) summarizes all SBDTs and the large-scale multi-tracer test started in 2017, allowing for a multi-scale interpretation of the groundwater protection area Donauried-Hürbe and answering the research questions 7 – 11 in detail.

Between 2016 and 2021, 17 different groundwater monitoring wells in the southwestern part of the groundwater protection area Donauried-Hürbe are tested with a total of 51 SBDTs. For these tests, mainly the new injection methods and devices developed in the first two studies of this thesis (***Chapter 2***, ***Chapter 3***) are used. The results show a wide range regarding the wells' connection to the aquifer or the conduit system, also differences over depth are observed within single wells. Test duration varies between less than 4 hours to more than 34 days. While vertical downward flow is documented in three out of the 17 wells, four wells show upward movement.

The findings of the borehole investigations are successfully used to verify the conceptual groundwater flow model of the groundwater protection area Donauried-Hürbe. Especially the vertical flow detected in the southern area of the Swabian Alb confirms the descent of groundwater under the younger Molasse sediments and ascending water in the area of the Danube valley.

For the southern part of the Swabian Alb, Kolokotronis et al. (2002) and Armbruster et al. (2008) assume mean residence times of 10 – 20 years based on isotope data, including a share of up to 30 % with more than 50 years. Also, a fast flow component with residence times of a few days is identified (Kolokotronis et al. 2002; Armbruster et al. 2008). The latter is confirmed by the sodium naphthionate breakthrough of the regional multi-tracer test, showing high flow velocities of up to 80 m/h between the swallow hole in the lone valley and the westernmost Nau spring group. These high velocities attest a highly karstified connection, however, the low recovery rate suggests other, most likely deeper flow paths.

With the eosin injection a fast flow connection (v_{max} = 26.12 m/h) towards a groundwater monitoring well is detected, but also a significantly delayed arrival at two nearby springs, Nauursprung spring and Öchslesmühlen spring. With first detections 250 and 307 days after the injection, maximum velocities of 0.44 and 0.39 m/h can be calculated. This discrepancy is caused by young, low permeable sediments blocking the karst conduits towards the spring. This leads to a still ongoing tracer breakthrough at both springs with low concentrations and a total recovery of around 8.5 to 9 % as of March 2023 concentrations that fluctuate at a low level. Due to the spring group's large catchment in combination with different inflow characteristics as well as the distance between the different springs and the sampling point, the concentration curve does not show any correlation with precipitation, sampling time or global radiation.

A comparable situation can be the reason that until March 2023, uranine is only detected in three monitoring wells southeast of the injection well. The missing detections in the production wells of the state water supply are to be seen positively regarding the effectiveness of the existing protection concept, especially with respect to the high-volume groundwater extraction. For all results of the multi-tracer test, the general low-flow conditions during the last years have to be taken into account.

To set the results obtained with the large-scale multi-tracer test into a regional context, other tracer tests in the surrounding area of the study site can be referred to. Kolokotronis et al. (2002) documented a total of 152 tracer tests conducted in the area of the eastern Swabian Alb. While 54 tracer tests remained without a detection at the sampling points, 98 tests led to at least one documented arrival at the observed springs or wells. In total, 246 breakthroughs were observed. Most of these tests focused on the examination of the Swabian Alb's Jurassic karst aquifer, only few tests over short distances were conducted solely in younger sediments (Kolokotronis et al. 2002). ***Figure 30*** compares the tracer tests from the literature with the results obtained by the multi-tracer test in the groundwater protection area Donauried-Hürbe.

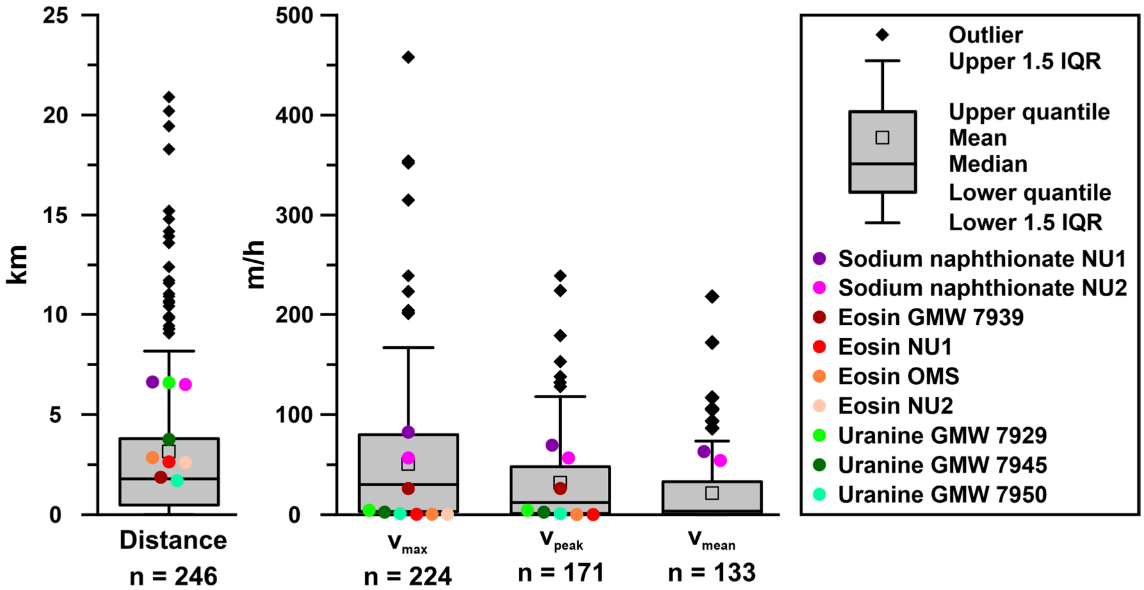

Figure 30: *Comparison of the results gained from the multi-tracer test (colored points) with other tracer tests (box plots) conducted in surrounding areas with comparable geology (Kolokotronis et al. 2002).*

The previous tracer tests documented flow connections with lengths between 0.5 and 4 km (Kolokotronis et al. 2002). The longest proved flow path extends over 20.9 km towards the Buchbrunnen spring in Dischingen, which is also used for drinking water supply. With around 6.5 km, the sodium naphthionate breakthrough at Nauursprung spring and the uranine detection in GWM 7929 also documented long flow paths.

With respect to the flow velocities, most values obtained in this thesis are located at the lower end of the available data set. For the eosin breakthroughs at the springs, the low-permeable sediments cause slow maximum velocities between 0.26 and 0.44 m/h. The velocities obtained from the uranine detections are also low due to a delayed transport into the high-flow conduit system. Only the highly karstified connection between the Lone swallow hole and Nauursprung spring leads to flow velocities above average. Overall, the earlier tests showed an even wider range of velocities than the multi-tracer test conducted in this study.

In conclusion, the applied methods are successfully used to document a distinct heterogeneity of groundwater flow in the catchment of the state water supply and, thus, are well-suitable for the characterization of complex aquifer systems. Regarding the conductivity scale effect (Kiraly 1975; Hartmann et al. 2014), the distribution of hydraulic conductivities can be documented with the selected methods from the scale of a single well up to the aquifer scale, which covers distances of several kilometers.

The documented flow paths and velocities can help the Zweckverband Landeswasserversorgung for the future management of the water resources and especially in case of a contamination. Also, for the hydrological conditions during the duration of the tracer test, the functionality of the existing protection concept was confirmed, since no fast flow towards the extraction wells was documented.

5.2 Outlook

Permeable injection bag method

The simplified method for uniform injection SBDTs developed within the scope of this thesis is already in use and will be used for further investigations, especially in the groundwater protection area Donauried-Hürbe, where, during a recent field test campaign as part of a bachelor thesis, multiple wells in the eastern part were characterized with SBTDs. The three big advantages, cost-efficiency, ease of use combined with little equipment as well as flexibility regarding the hydrogeological setting leads to a wide range of possible applications. The method is especially predestined for areas where a large number of boreholes or groundwater monitoring wells are to be tested, for example, contamination sites where the depths of the major flow horizons must be known to estimate the dispersal of the pollutants (Bear et al. 1993; Berkowitz 2002; D'Affonseca et al. 2008).

With the current state of SBDT methods, it is difficult to gain reliable filtration velocities if the permeabilities of the surrounding aquifer are unknown, since the required correction factor α (Equation 10) cannot be determined. Further tests in different geological formations could address this problem by creating a larger data set that can be compared with the results of other methods, for example pumping tests. This could enable the calculation of filtration velocities and would lead to a better quantitative evaluation of SBDTs.

Point injection probe

The point injection probe was already used for further investigations in the groundwater protection area Donauried-Hürbe. Especially, a 110 m deep well with multiple filter zones in an area with expected ascending groundwater was examined with point injections. For such deep wells, the new injection probe could be further developed, since vertical flow might vary over depth due to multiple in- and outflow horizons. This could be investigated by multiple consecutive point injections, which, however, can require a long time, depending on the well's outflow behavior and flow velocities. As an alternative the depth dependence of vertical groundwater flow could be investigated with only one test, by connecting two or more injection probes in series, which allow for a simultaneous multi-point injection. Technically, this could be achieved by another falling weight connected to the casing of the upper probe that is released during the opening process and triggers the mechanism of the lower probe.

Multi-scale aquifer characterization using tracer methods

With the applied methods, a multi-scale aquifer characterization was achieved. However, to gain even more information on an aquifer system, an additional tracer method could be used. Natural tracers, typically major ions, trace elements or water isotopes, can be used to investigate and characterize aquifer systems, sub-catchments, residence times and mixing processes (Goldscheider and Drew 2007; Barberá and Andreo 2012; Ravbar et al. 2012; Mudarra et al. 2014b; Hartmann et al. 2014). Natural tracers can also provide information on dissolution processes and flow paths (Frank et al. 2019).

Suitable natural tracers are dependent of the respective system. In the groundwater protection area Donauried-Hürbe, nitrate could be used as well as present trace elements or isotopes. With the help of natural tracers, the sub-catchments of the six well fields and the Nau springs in Langenau could be investigated to complement the results of the SBDTs and the multi-tracer test.

Groundwater protection area Donauried-Hürbe

In the complex aquifer system in the groundwater protection area Donauried-Hürbe, many questions are still unanswered, since the conducted multi-tracer test focused on the western part of the catchment. To complement the results obtained in this thesis, a second multi-tracer test in the eastern part of the catchment is currently being planned in detail. Potential injection points in the eastern part were already identified during the preparation of the first tracer test.

Another Lone swallow hole, around 10 km east-northeast of the previous injection point in the Lone valley, is one intended tracer injection point. Due to a wastewater treatment plant, a potential contamination risk is present at this site, which is why the flow times towards the extraction wells are highly relevant for the state water supply. The outflow of the wastewater treatment plant provides a constant discharge, but the riverbed in front of the swallow hole is obstructed with several beaver dams that will complicate the injection. A second promising injection point is a swallow hole with continuous discharge in a doline just 2.5 km north of one of the state water supply's well fields. At this site, the drainage of a nearby road and a biogas plant pose an increased contamination risk.

For the detailed planning, the results and experiences of the first tracer test can provide a valuable basis. Since at both sites tracer will be injected in naturally developed swallow holes with continuous flow, fast connections with velocities comparable to the sodium naphthionate breakthrough are possible, which has to be considered for the sampling campaign. In order to prepare the sampling program, several karst GMWs between the injection points and the extraction wells in the Danube valley were already examined with SBDTs. Based on these results, the target depths for water samples and activated charcoal adapters can be defined.

Even though the injection sites are east of Langenau, an arrival at the Nau springs cannot be excluded, which is why the discharge monitoring of the springs should be improved for the second tracer test. Promising tests in 2019 used an OTT SVR for radar-based measurements of flow velocities at the water surface to calculate the discharge at one sampling point (Siedschlag 2019). To obtain continuous discharge data, the relation of discharge and flow velocity must be known. This can be achieved with multiple measurements during changing conditions using an acoustic or electrical-inductive flow meter, for example an OTT ADC (Song et al. 2012) or a classical current meter.

In addition to the second tracer test, a repetition of the previous tracer injections under different hydrological conditions would be interesting. Especially the connection between the Lone swallow hole and Nauursprung spring could lead to even faster flow velocities during high-flow conditions and could therefore be used to approach the maximum velocities of the system.

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DECLARATION OF AUTHORSHIP

Study 1


Hydrogeology Journal

REPORT

Comparative application and optimization of different single-borehole dilution test techniques

Abstract

Introduction

Citation: *Fahrmeier, N., Goeppert, N., Goldscheider, N. (2021) Comparative application and optimization of different single-borehole dilution test techniques. Hydrogeology Journal 29:199-211. https://doi.org/10.1007/s10040-020-02271-2*

Declaration of authorship: The idea for the method was developed by all authors. Nikolai Fahrmeier (NF) conducted the field tests, processed the data in consultation with Nadine Goeppert and Nico Goldscheider. The manuscript was written by NF and reviewed and edited by all authors.

Study 2


Hydrogeology Journal

TECHNICAL NOTE

A novel probe for point injections in groundwater monitoring wells

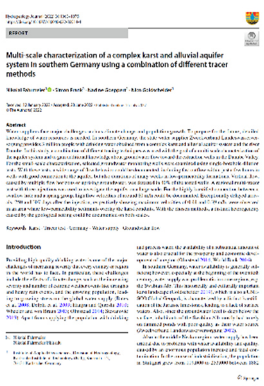
Abstract

Introduction

Citation: *Fahrmeier N, Goeppert N, Goldscheider N (2022) A novel probe for point injections in groundwater monitoring wells. Hydrogeology Journal 30:1021–1029. https://doi.org/10.1007/s10040-022-02477-6*

Declaration of authorship: The injection probe was developed by Nico Goldscheider and NF. The field and laboratory tests were conducted by NF. All authors substantially contributed to editing and reviewing the manuscript.

Study 3


REPORT

Multi-scale characterization of a complex karst and alluvial aquifer system in southern Germany using a combination of different tracer methods

Abstract

Introduction

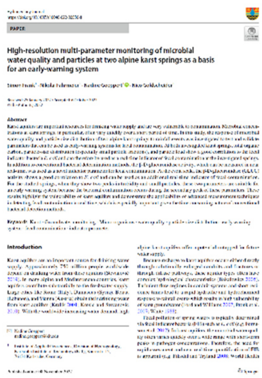
Citation: *Fahrmeier N, Frank S, Goeppert N, Goldscheider N (2022) Multi-scale characterization of a complex karst and alluvial aquifer system in southern Germany using a combination of different tracer methods. Hydrogeology Journal 30:1863–1875. https://doi.org/10.1007/s10040-022-02514-4*

Declaration of authorship: All authors were involved during the planning of the field work, which was conducted by NF and Simon Frank. NF wrote the initial draft and all authors reviewed and edited the manuscript.

Patent Point Injection Probe

Declaration of inventorship: Nico Goldscheider, Nikolai Fahrmeier and Nadine Goeppert are equal inventors of the probe.

Study 4 (not included in this thesis)


PAPER

High-resolution multi-parameter monitoring of microbial water quality and particles at two alpine karst springs as a basis for an early-warning system

Introduction

Citation: *Frank S, Fahrmeier N, Goeppert N, Goldscheider N (2022) High-resolution multi-parameter monitoring of microbial water quality and particles at two alpine karst springs as a basis for an early-warning system. Hydrogeology Journal. https://doi.org/10.1007/s10040-022-02556-8*

Declaration of authorship: Simon Frank and NF conducted the field work and processed the data, which was discussed and evaluated by all authors. Simon Frank wrote the manuscript, which was reviewed and edited by all authors.

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