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Combining measurements, remote sensing and numerical modelling to assess multi-scale flow dynamics in groundwater-dependent environmental systems

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M.Sc. Erik Nixdorf

Geboren am 16.01.1988 in Burg

Gutachter:

Prof. Dr. Olaf Kolditz, Technische Universität Dresden

Prof. Dr. Beidou Xi, Chinesische Forschungsakademie der Umweltwissenschaften Peking

JProf. Dr. Marc Walther, Technische Universität Dresden

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Leipzig, Mai 2018

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Leipzig, Mai 2018

Erik Nixdorf

Abstract

Groundwater flow modelling provides an important quantitative instrument for addressing issues related to the quantity and quality of groundwater and the connected water resources. Consequently, groundwater flow models have been developed and used ubiquitously in science to deepen the understanding of subsurface processes and their drivers as well as management and planning tools.

The present work investigates how numerical models can be linked to field investigations and public databases to quantitatively approach questions in the area of groundwater research. The primary goal is to develop new, efficient ways to overcome limitations of the individual hydrological concepts for solving specific hydrological problems and to increase the understanding of practical applicability of different methods. For this purpose, tailor-made approaches were developed for different study areas covering diverse spatial scales: the hydrology of a small mining lake, the riparian aquifer at the scale of a single meander as well as the aquifer systems of a large-scale river basin in China.

The first part of the work deals with the physical and mathematical modelling of water constituents balance in a meromictic mining lake in Lusatia. The capability of using a rather simple mass-balance model based on a sufficient dataset of field data to evaluate lake stratification and lake-groundwater interaction were shown.

In the second part, a transient numerical groundwater flow model was developed for the riparian aquifer of a stream meander and was calibrated by three different salt tracer tests. The model was used to proof the reliability of subsurface travel times derived from time series analysis and to give insights in the riparian zone dynamics during changing hydraulic gradients.

The third part of the work describes the methodology to conduct risk assessment of groundwater contamination on the large catchment scale of the Songhua River in China. A comprehensive literature study was conducted to get an overview about measurement data on water quality data in China. A three-dimensional numerical flow and mass transport model was applied to access the flow and matter transport dynamics in the aquifer system of a sub-basin considering changing groundwater exploitation scenarios. Consequently, numerical groundwater modelling was combined with processed remote sensing and web mapping

service data to overcome field data limitations and to derive groundwater vulnerability, groundwater hazard and groundwater risk maps for the entire Songhua River Basin.

Summarizing, this doctoral thesis could develop new methods of combining field measurements, data assimilation and aggregation from various sources and groundwater modelling strategies and successfully apply these methods to find solutions on problems of multiple scales and across water systems.

Kurzfassung

Die Grundwassermodellierung stellt eine wichtige wissenschaftliche Methode zur quantitativen Analyse von Fragestellungen zum Schutz der Menge und Güte der Grundwasserressourcen sowie der angeschlossenen Wasserkörper dar. Dementsprechend werden Grundwassermodelle sowohl für Planungs- und Bewertungszwecke im Wasserressourcenmanagement als auch zur wissenschaftlichen Erforschung der Prozesse im Untergrund entwickelt und angewendet.

Die vorliegende Arbeit untersucht in diesem Rahmen, wie numerische Modelle, Feldmessungen und Daten generiert aus Fernerkundungsdaten und Webplattformen systematisch verknüpft werden können, um Fragestellungen im Bereich der Grundwasserforschung quantitativ zu beantworten. Das Ziel der Arbeit ist es neue effiziente Abläufe zu entwickeln, die die Limitierung der einzelnen Methoden überwinden und diese auf deren Anwendbarkeit für die Lösung spezifischer hydrologischer Probleme zu analysieren. Zu diesem Zweck wurden in dieser Doktorarbeit fallspezifische Lösungen für verschiedene Untersuchungsgebiete entwickelt, die sowohl in der räumlichen Skale als auch in den zu untersuchenden hydrologischen Fragestellungen eine große Diversität aufweisen.

Im ersten Teil der Arbeit wurde die Massenbilanz von Wasserinhaltsstoffen in einem meromiktischen Tagebaurestsee im Lausitzer Revier durch physikalische und mathematische Modellierungsmethoden untersucht. Dabei konnte gezeigt werden, dass auf Basis einer gewonnenen mehrjährigen Zeitreihe von Messdaten ein einfaches Massenbilanzmodell in der Lage ist, sowohl Seeschichtungs- als auch Grundwasseraustauschdynamiken quantitativ zu beschreiben.

Der zweite Teil der Arbeit umfasst die Entwicklung eines transienten numerischen Grundwassermodells für den quartären Uferaquifer im Bereich eines Flussmäanders der Selke welches anhand von Daten aus mehreren Salztracertests kalibriert wurde. Das Modell wurde dafür verwendet die transienten Verweilzeiten in der gesättigten Zone des Mäanderbogens unter dem Einfluss dynamischer hydraulischer Bedingungen zu untersuchen. Die Ergebnisse wurden im Anschluss mit Verweilzeiten verglichen, die aus der Analyse der zeitlichen Verschiebung von gemessenen elektrischen Leitfähigkeitszeitreihen zwischen Fluss und Grundwassermessstellen gewonnen wurden. Durch dieses kombinierte Verfahren konnten sowohl die Beschränkungen der zeitreihenbasierten Verweilzeitberechnung aufgezeigt als

auch ein tieferes Systemverständnis für die Interaktionsdynamiken zwischen Grund- und Flusswasser auf der Mäanderskala gewonnen werden.

Der dritte Teil der Arbeit beschreibt die Vorgehensweise für die Bewertung des Grundwasserkontaminationsrisikos im Einzugsgebiet des Songhua Flusses in China. Eine umfassende Literaturstudie wurde durchgeführt, um einen Überblick über die Verfügbarkeit von Messdaten zur Belastung der Wasserressourcen Chinas mit organischen Schadstoffen zu erhalten. Danach wurde für ein Teileinzugsgebiet ein dreidimensionales numerisches Grundwassermodell auf Basis der vorhandenen hydrogeologischen Daten aufgebaut. Dieses wurde dazu verwendet die Änderungen im Stofftransports und den Schadstoffkonzentrationen innerhalb des Aquifersystems unter steigenden Entnahmeraten zu analysieren. Basierend auf diesen Studien wurden auf der Skale des Gesamteinzugsgebiets, um die beschränkte Verfügbarkeit von Felddaten auszugleichen, die Ergebnisse der numerischen Grundwassermodellierung mit Fernerkundungsdaten und Webdatenbanken in einem Indexsystem kombiniert mit dem für die oberflächennahen Aquifere Vulnerabilität, Gefährdungspotential und Verschmutzungsrisiko in einer räumlichen Auflösung von 1 km² bestimmt wurden.

Zusammenfassend konnten durch die vorliegende Doktorarbeit neue passgenaue Methoden zur effektiven Kombination von in-situ Messungen, der Datenerhebung und Datenintegration aus vielfältigen Datenquellen sowie numerischen Grundwassermodellierungsstrategien entwickelt und zur Lösung der untersuchten hydrologischer Fragestellen auf den verschiedenen Skalen und über die Grenzen der einzelnen hydrologischen Teilsysteme hinaus erfolgreich angewandt werden.

Theses

1. Time series of electrical conductivity (EC) profile measurements provide a useful metric to derive the total amount, distribution and dynamics of electro-active water constituents in iron-meromictic mining lakes. The total amount of electro-active species resembles the seasonal changes in volume ratio between the oxygenated mixolimnion and the anoxic monimolimnion.
2. A simple mass balance model including mixing and re-dissolution processes is able to show that internal biogeochemical processes are able to sustain the iron meromixis in the investigated mining lake. However, due to the incomplete re-dissolution of precipitated iron-hydroxide flocs in the monimolimnion, the exchange with ion-rich ambient groundwater is the main driver stabilizing the stratification over the course of several years.
3. Mixolimnectic and monimolimnetic water of iron-meromictic lakes could both originate from the same source. Following aeration, monimolimnetic water undergoes chemical changes and approximates the chemical properties of mixolimnetic water.
4. The application of electrical conductivity time series to estimate riparian travel times is limited, particularly for EC fluctuations caused by storm events. Estimated travel times can result in negative values, even if losing conditions prevail over the investigation time. The main reason is the mobilization of pre-stored groundwater in the riparian aquifer due to changing hydraulic gradients.
5. Combining a numerical groundwater flow model transiently calibrated to salt tracer tests with numerical particle tracking is an adequate approach to assess the flow field dynamics in the riparian zone of a river meander. Using backward-in-time numerical particle tracking enables proofing the plausibility of travel time estimates from the time series analysis.
6. In the absence of induced infiltration by groundwater extraction, high hydrograph and chemograph slopes during an event are an important prerequisite for the successful application of cross-correlation analysis of EC data to estimate riparian travel times.
7. For the study area of Acheng City, a three-dimensional numerical flow and matter transport model provides an appropriate tool to forecast the impact of increased groundwater abstraction on the extent of flow path inversion and the acceleration of

flow velocities in the aquifer surrounding of the well fields. It further allows identifying the risk of drinking well pollution by contamination from industrial sources.

8. Integrating numerical modelling, public datasets and web mapping services into an index-based groundwater risk assessment framework is an appropriate approach to overcome data limitations for groundwater risk assessment of large basins. In particular, web mapping services in combination with a hazard classification system are able to establish a comprehensive hazard inventory independently of the availability of cadastral data.
9. The application of the methodology to the Songhua River Basin demonstrated that groundwater vulnerability and pollution risk of a significant part of the catchment's plain areas is emphasized. Higher hazard potential tends to be associated with higher groundwater vulnerability.
10. The sole requirements for the developed risk assessment approach are publicly available datasets and open source software, which ensure its reproducibility and allows it to be transferable to assess the groundwater risk in other catchments in China and the world with limited access to field data.

Thesen

1. Gemessene Zeitreihen von elektrischen Leitfähigkeitsprofilen stellen einen geeigneten Parameter dar, um die Gesamtmenge, Verteilung und Dynamik der gelösten Stoffe in eisenmeromiktischen Tagebaurestseen zu beschreiben. Die Gesamtmenge der gelösten Stoffe folgt den saisonalen Änderungen im Volumenverhältnis zwischen dem oxischen Mixolimnion und dem anoxischen Monimolimnion.
2. Mit Hilfe eines auf EC-Profildaten basierenden Massenbilanzmodells, welches sowohl partielle Durchmischungs- als auch Rücklösungsprozesse abbildet, kann nachgewiesen werden, dass interne biogeochemische Prozesse in der Lage sind die Meromixis zu erhalten. Da die Rücklösung der ausfallenden Eisenhydroxidflocken nur unvollständig stattfindet, ist der Austausch mit ionenreichen Grundwasser entscheidend für die Stabilisierung der Schichtung über längere Zeiträume.
3. Sowohl das Wasser aus dem Mixolimnion als auch aus dem Monimolimnion können denselben Ursprung haben. Durch Belüftung nähern sich die hydrochemischen Eigenschaften des monimolimnetischen Wassers denen im Mixolimnion an.
4. Die Anwendung von Zeitreihen der elektrischen Leitfähigkeit zur Bestimmung von Fließzeiten im Uferaquifer durch die Kreuzkorrelationsanalyse ist beschränkt, insbesondere für den Fall, dass die Fluktuationen im EC-Signal auf kleinere natürliche Hochwasserereignisse zurückgehen. In diesem Fall kann die Zeitreihenanalyse zur Berechnung negativer Fließzeiten zwischen Fluss und Grundwassermessstelle führen, auch wenn infiltrierende Austauschbedingungen über den gesamten Messzeitraum vorliegen. Die Hauptursache dafür liegt in der Mobilisierung von Grundwasser im Uferaquifer aufgrund der sich verändernden hydraulischen Gradienten.
5. Ein transientes numerisches Grundwassermodell in Kombination mit numerischer Partikelrückverfolgung, welches an Hand von Salztracertests kalibriert wird, stellt ein geeignetes Verfahren dar, um die Dynamiken im Strömungsfeld des ufernahen Grundwasserleiters abzubilden. Die Nutzung von numerischer Partikelrückverfolgung ermöglicht es, die mit Hilfe der Zeitreihenanalyse gewonnen Fließzeiten auf ihre Plausibilität zu überprüfen.
6. Starke Gradienten im Hydrographen und Chemographen eines Ereignisses sind eine wichtige Voraussetzung für die erfolgreiche Anwendbarkeit der EC Zeitreihenanalyse

zur Bestimmung der Fließzeiten im ufernahen Grundwasserleiter, insbesondere wenn keine aktiven Grundwasserfassungen vorliegen.

7. Für das Untersuchungsgebiet in der Umgebung der Stadt Acheng kann durch ein dreidimensionales transientes Grundwassermodell der Einfluss von steigenden Grundwasserentnahmeraten auf die Ausbreitung des Absenktrichters und die Änderungen der Fließgeschwindigkeiten im Bereich der Brunnenfelder prognostiziert werden. Darüber hinaus kann mit Hilfe des Modells die zukünftige Gefährdung der Trinkwassergewinnung durch Altlasten in den lokalen Industriegebieten abgeschätzt werden.
8. Die Integration von numerischer Grundwassermodellierung, öffentlichen Datensätzen und Webmapping-Diensten in ein indexbasiertes Bewertungsschema stellt eine geeignete Methode zur Abschätzung des Grundwasserrisikos auf großen Skalen dar. Insbesondere die Kombination von Daten aus Webmapping-Diensten mit einem Gefahrenklassifierungssystem ermöglicht es einen räumlich hochaufgelösten Gefährdungskatalog für den zu untersuchenden Grundwasserkörper zu erstellen ohne auf Katasterdaten zurückgreifen zu müssen.
9. Die Anwendung dieses Ansatzes zur Grundwasserrisikoabschätzung auf das Einzugsgebiet des Songhua Flusses zeigt, dass sowohl die Vulnerabilität als auch das Verschmutzungsrisiko für einen großen Teil der Grundwasserkörper in der Songnen-Ebene erhöht ist, insbesondere in der Nähe der größeren Siedlungsgebiete wie Changchun. Dabei kann eine räumliche Korrelation zwischen Gebieten mit erhöhter Vulnerabilität und einem erhöhtem Gefährdungsrisiko nachgewiesen werden.
10. Die ausschließliche Nutzung von freizugänglichen Datensätzen für den entwickelten Ansatz zur Bestimmung des Grundwasserrisikos gewährleistet dessen Transparenz und Nachvollziehbarkeit. Darüber hinaus ermöglicht die entwickelte Methodik, auch das Verschmutzungsrisiko für andere Grundwasserkörper in China oder auch weltweit abzuschätzen, insbesondere wenn der Zugang zu Felddaten eingeschränkt ist.

List of publications

ISI PUBLICATIONS

Nixdorf E, Sun Y, Lin M, Kolditz O. 2017. Regional assessment of groundwater contamination risk in the Songhua River Basin, China, by integrating public data sets, web services and numerical modelling techniques. Science of the Total Environment 605:598-609 DOI: 10.1016/j.scitotenv.2017.06.126

Nixdorf, E., Trauth, N., 2018. Evaluating the reliability of cross-correlation method to estimate riparian travel times under time variant hydraulic gradients. Hydrol. Process. 32 (3): 408-420 DOI: 10.1002/hyp.11428

Nixdorf E, Boehrer B. 2015. Quantitative analysis of biogeochemically controlled density stratification in an iron-meromictic lake. Hydrology and Earth System Sciences 19 (11): 4505–4515 DOI: 10.5194/hess-19-4505-2015

Nixdorf E, Chen C, Sun Y, Kolditz O. 2015. Persistent organic pollutants contaminate Chinese water resources: overview of the current status, challenges and European strategies. Environmental Earth Sciences 74 (2): 1837–1843 DOI: 10.1007/s12665-015-4448-x

OTHER PUBLICATIONS

Sachse A, **Nixdorf E**, Jang E, Rink K, Fischer T, Xi B, Beyer C, Bauer S, Walther M, Sun Y, et al. 2017. OpenGeoSys-Tutorial: Computational Hydrology II: Groundwater Quality Modeling. Springer. DOI: 10.1007/978-3-319-52809-0

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Chen C, Börnick H, Cai Q, Dai X, Jähnig S, Kong Y, **Nixdorf E**, Krebs P, Kuenzer C, Kunstmann H, et al. 2015. Challenges and opportunities of German-Chinese cooperation in water science and technology. Environmental Earth Sciences 738 (8):4861-4871 DOI: 10.1007/s12665-015-4149-5

Mao L, Danfeng J, Chifei C, Sun Y, Su J, Xi B, **Nixdorf E**. 2016. Groundwater Vulnerability Partition in Ashi River Basin. Research of Environmental Sciences 29 (12): 1773–1781 (in Chinese) DOI: 10.13198/j.issn.1001-6929.2016.06

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Contents

List of figures

1. General introduction

1.1 Motivation

Groundwater is one of the most valuable natural resources with an outstanding importance for ecological diversity, human health as well as global energy and food security. Considering that it is the largest share of unfrozen freshwater on earth and has inherent qualities in terms of accessibility, availability and its susceptibility to pollution, groundwater is in many areas of the world the most important source for drinking water supply (Aeschbach-Hertig and Gleeson, 2012). The largest share of groundwater is utilized for irrigation, which means that a considerable amount of the global food production rely on the availability of non-polluted groundwater resources (Siebert et al., 2010).

Despite their vital importance for the population, groundwater resources are unsustainably managed in many parts of the world. The availability of motor driven pumps led to a tremendous increase of groundwater exploration followed by continues groundwater depletion in many areas of the globe (Konikow and Kendy, 2005; Famiglietti, 2014). Important examples for overexploited large aquifers are the aquifer system of the Indo-Gangetic Plain (Rodell et al., 2009) and the aquifers in the northern and western parts of China (e.g. Feng et al., 2013; Chen et al., 2016). In addition, a multitude of groundwater resources are not only running short but are also polluted continuously, which cause serious health risks to both man and animals. Groundwater contamination covers a broad range of contaminant classes and source types and depends on the location. For instance, fertilizer inputs from diffusive agricultural sources as well as organic pollutants from active industrial sources and brownfields cause increasing groundwater contamination in many different countries of the world such as Germany (Salomon et al., 2016) and China (Zhai et al., 2017). On the other hand, groundwater pollution with substance such as Arsenic (Alam et al., 2002) or acidic mine drainage (Rolland et al., 2001) have a high importance for specific areas on a regional or local level.

The task of protecting the groundwater resources faces not only governmental authorities to develop comprehensive strategies of groundwater management (Aeschbach-Hertig and Gleeson, 2012) but also calls upon science to derive and provide information, to develop solutions and to forecast consequences for groundwater related problems (Liu et al., 2008) cooperatively together with other stakeholders (Cosgrove and Loucks, 2015). In this context, mathematical groundwater flow models are applied as one method to provide a quantitative framework for answering questions about groundwater flow systems and management strategies of groundwater resources (Anderson et al., 2015). Over the last decades, the tremendous increase in available computational power and improved programming languages (Hayley, 2017) promoted the development of process-based numerical groundwater flow models to simulate e.g. stationary or transient multi-process flow (e.g. Walther et al., 2014; Trauth et al., 2014) across several dimensions and up to regional flow scales (e.g. Zhou and Li, 2011; Maheswaran et al., 2016). In this context, numerical groundwater models are able to cover heterogeneous media (e.g. Jang et al., 2017; Yang et al., 2015) and complex boundaries (e.g. Walther et al., 2017). Additionally, bibliographic studies give a quantitative proof (Fig. 1.1) that the amount of publications, which is assumed to correlate with the amount of research activities, on groundwater flow modelling is continuously increasing, particularly in developing countries such as China.

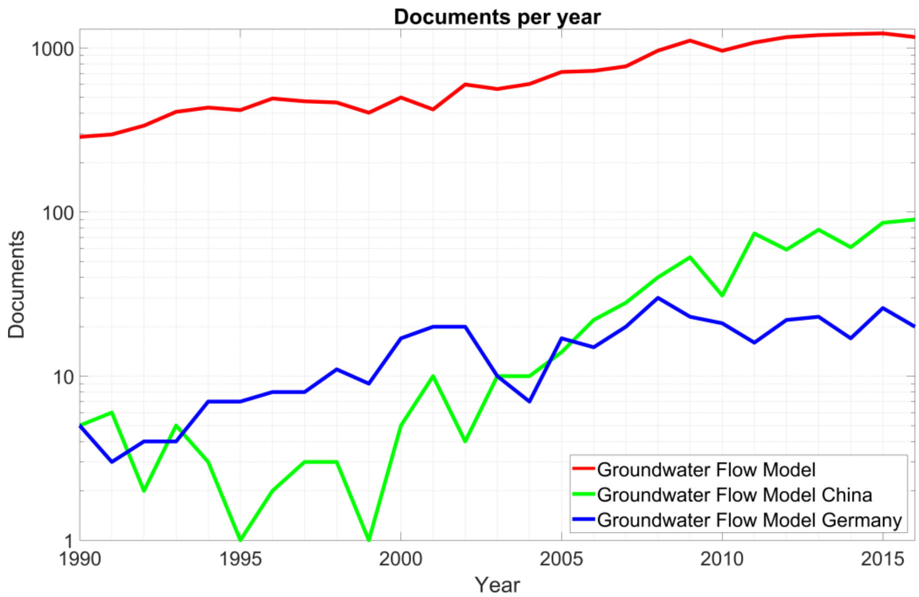

Figure 1.1: Scientific publications per year listed in the SCOPUS database from 1990 to 2016. The names of the graphs refer to the applied search terms. Search results were restricted to the fields "Article title, Abstract and Keywords".

In consequence, the continuous supply of state-of-the-art numerical models and their sophisticated graphical modules have made them a must-have item for hydrological studies (Vidon, 2015). On the contrary, this emphasize on numerical flow modelling in hydrology and water resources management is seen critical and state-of-the-art numerical flow models have been criticized for overlooking input data gaps (Silberstein, 2006), having theoretical constraints (Clark et al., 2016), overselling performance (Andréassian et al., 2007) as well as for being over-parametrized mathematical marionettes (Kirchner, 2006).

The methodological framework developed by this doctoral thesis aims to show exemplarily how to overcoming the division in hydrological science between experimentalists and modellers (Silberstein, 2006) by linking new data networks, field observations, field experiments and models on different scales to get new insights into the specific hydrological systems.

1.2 Structure

The dissertation is organized in three main sections covering the different study areas where groundwater is interacting with different parts of the connected hydrosystems (Fig. 1.2). The first two sections refer each to a corresponding publication in an ISI listed journal. In the third section, two ISI-listed publications are summarized together with a related part from a book publication at Springer and a publication in a domestic Chinese journal. The chapters are arranged chronologically following the methodological development of the doctoral thesis.

The first chapter contains investigations of the hydrochemistry in a permanently stratified mining lake interacting with the ambient groundwater. The focus of this study centered on the analysis of long term measurements of electrical conductivity (EC) profiles in Lake Waldsee by mass-balance modelling in combination with physical modelling of the lake in the laboratory.

In the following chapter, the previous made experiences with EC measurements and time series analysis at the mining lake were transferred to a study site at a German low land river. High-resolution EC time series were obtained in the stream and in a number of hydrologically connected monitoring wells and their fluctuations due to event driven river stage changes were analysed by windowed cross-correlation. The reliability of the derived travel-time characteristics was proved by developing and applying a transient numerical groundwater flow model in combination with an advective particle-tracker on the investigated part of the riparian aquifer.

In chapter 4, the gained knowledge in modelling and measuring techniques was utilised to analyse the risk of groundwater being polluted by chemicals in the study area of the Songhua River Basin in China. First, a comprehensive bibliographic study was conducted to assess the availability of water quality data in China. A process-based hydrochemical numerical groundwater flow model was developed for a smaller sub-catchment to determine potential threats for the local water supply system. Taking into account that a dense network of hydro(geo)logical data and groundwater quality measurements are not accessible on the basin scale, a new hybrid approach between index and processed based groundwater risk assessment techniques was developed by applying remote sensing data, public sets of reanalyzed data, numerical groundwater flow model results and web mapping service data collectively. The spatial distribution of groundwater risk was assessed and parameter sensitivities and uncertainties were analysed.

Consequently, the main results of the individual chapters were summarized and concluded to a broader perspective. Finally, recommendations for future work were given based on limitations of the used approaches.

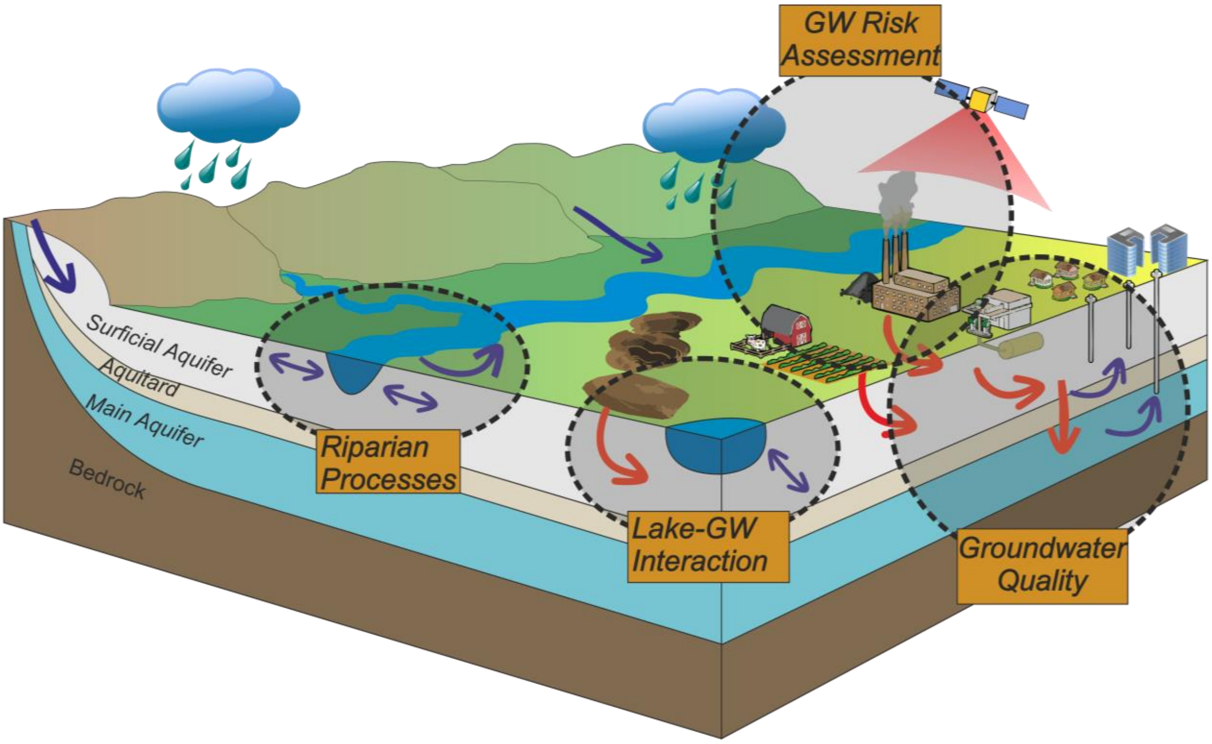

Figure 1.2: Conceptual drawing of interconnected hydrological processes investigated within this doctoral thesis. The blue arrows show exchanging water fluxes between different compartments and the red arrows indicate matter fluxes of potentially hazardous substances. Double arrows indicate the fluxes for which directional changes were considered within the investigations. The individual topics of the thesis are encircled with black lines within the figure. The topic "Mining Lake Hydrology" refers to chapter 2, "Surface Water–Groundwater Interaction" is addressed in chapter 3 and the topics "Groundwater Risk Assessment" and "Groundwater Quality" are subject of chapter 4 of this doctoral thesis.

2. Quantitative analysis of biogeochemically controlled density stratification in an iron-meromictic lake

The content of this chapter is included in:

Nixdorf E, Boehrer B. 2015. Quantitative analysis of biogeochemically controlled density stratification in an iron-meromictic lake. Hydrology and Earth System Sciences 19 (11): 4505–4515.

Nixdorf E, Boehrer B. 2016. Biogeochemical processes controlling density stratification in an iron-meromictic lake. In IMWA 2016 – Mining Meets Water – Conflicts and Solutions, Drebenstedt C., Paul M. (eds).TU Bergakademie Freiberg): Freiberg/Germany; 269–275.

In many mining regions on earth, pit lakes have been identified where a permanent stratification creates an anoxic reductive deep water layer, the monimolimnion, with increased concentrations of dissolved gases and undesired ionic substances, e.g. heavy metals (Boehrer and Schultze, 2008). Typically meromictic conditions in mining lakes are sustained by a continuous inflow of denser groundwater and surface water via streams or precipitation and the very low diffusion rate of substances via the zone of sharp gradients (von Rohden and Ilmberger, 2001). Additionally, chemical reactions are able to sustain meromixis in lakes, e.g. the removal of iron from the upper water by oxidation and precipitation (Boehrer et al., 2009). It is also known that re-dissolution of iron occurs in the deep water, but there has not been any quantitative approach to determine its role in sustaining meromixis.

In this study, a new quantitative approach was developed to access the contribution of chemical reactions and exchange fluxes sustaining the density stratification. As an example, the prominent case of iron meromixis in Waldsee near Doebern was chosen, a small pit lake supplied by groundwater inflow with an area of about 2400 m² and a maximum water depth of 4.7 m (Boehrer et al., 2009). The physico-chemical profiles of Waldsee show a strong discrepancy in water parameters between the upper 1-1.5 m thick oxygenated mixolimnic water layer and the higher mineralized monimolimnion below. The boundary layer between both layers, the chemocline, varies with amplitude up to 1 m due to seasonal changes.

The objectives of the investigations were:

1) Quantify the amount and the dynamics of electro-active species in Lake Waldsee and its water layers

2) Proof the relevance of the proposed hydrochemical system controlling mass balance and stratification in the lake
3) Evaluate the impact of continuous groundwater recharge on lake stratification

Monthly measured high temporal resolution electrical conductivity (EC) profiles from a four-year data set were integrated over the corresponding lake volume layers to derive the quantitative variable summed conductivity as a parameter reflecting the amount and seasonal mass-balance dynamics of electro-active substances in the entire lake:

$$S_{\kappa_{25}}\left(t_i\right) = \sum_{j=1}^{n} \kappa_{25}\left(j, t_i\right) \cdot V_j = \sum_{j=1}^{n} \kappa_{25}\left(j, t_i\right) \cdot A_j \cdot h_j \qquad (1)$$

Where $S_{\kappa 25}$ is the summed conductivity [S/m²], κ_{25} is the electrical conductivity corrected for a temperature of 25°C [mS/cm], t_i is the time at timestep i, j is the individual layer of the lake and h_j, A_j and V_j are height, planar area and volume of the corresponding layer j.

Beside the assessment of the parameter summed conductivity for the entire water body, calculating the spatially averaged conductivity of mixolimnion and monimolimnion for each time step was used to quantify changes in stratification stability. Discrepancies between the measured dynamics of monimolimnion and mixolimnion conductivities and values calculated using a hypothetical scenario of a closed Waldsee (Fig. 2.1) represent the impact of cross-boundary mass fluxes on the electro-active species mass balance of Waldsee.

In addition, a column experiment was designed to replicate proposed dominating geochemical processes in Waldsee, foremost the iron-redox-cycle. Monimolimnetic water from Waldsee was filled in a 5 m high PVC column and partially aerated to remove iron compounds and organic material from the upper part of the column. Samples were taken from the water column after ceasing the aeration and the physicochemical water properties were analysed and compared with samples from the lake.

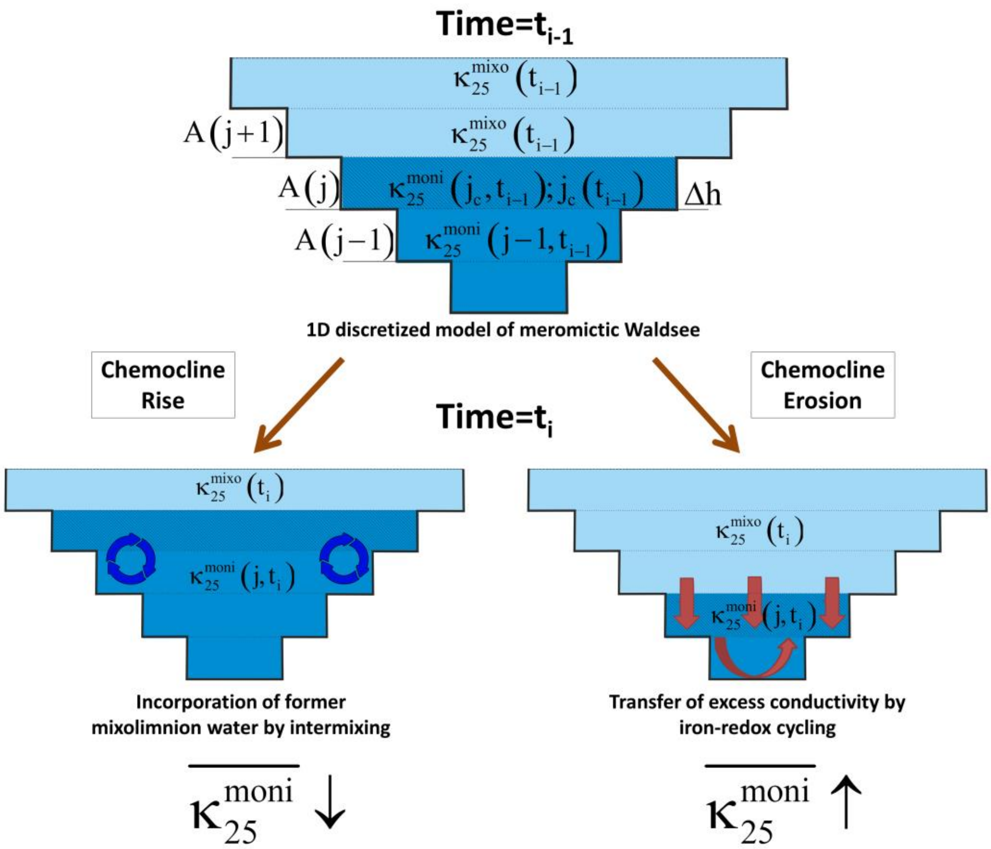

Figure 2.1: Conceptual model representing mass-balance dynamics in a hypothetical Waldsee without cross-boundary fluxes. Top: Discretization of Lake Waldsee into layers representing the shallow (light blue color) or deeper (dark blue color) section of Waldsee at a certain time step. Bottom: Depending on the chemocline position, either mixing processes or iron re-dissolution is able to change κ_{25} in the monimolimnion in accordance to the chosen modelling approach.

It could be shown that the calculated “summed conductivity” parameter followed the changing chemocline height with an increase of monimolimnion volume in winter and early spring and a decrease in the remaining months (Fig. 2.2). This means that the total amount of electro-active substances in Waldsee correlates significantly with the volume of the monimolimnion with variations up to 25 % within the observation period. Coinciding changes of average κ_{25} in the monimolimnion indicated that a considerable share of precipitated substances re-dissolved in the remaining anoxic deep waters and contributed considerably to the density stratification. This was confirmed by the column experiment where immediate precipitation of iron hydroxide flocks after the beginning of the aeration from the upper part of the column led to an approximation of EC, dissolved iron and dissolved organic carbon towards the mixolimnion value of Waldsee (Fig. 2.3).

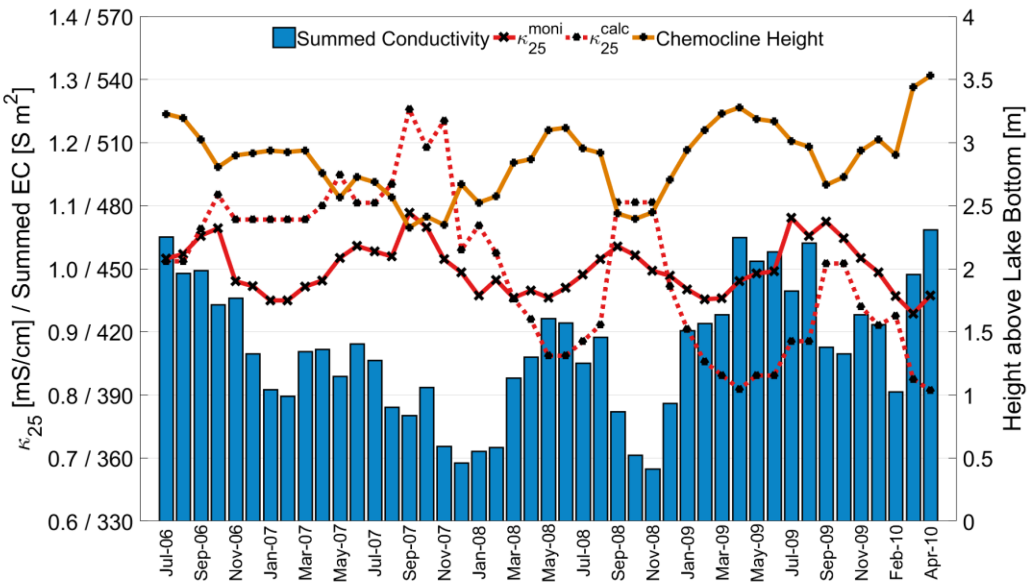

Figure 2.2: Time series of monthly chemocline height, summed EC and monimolimnetic κ_{25} in Waldsee between July 2006 and April 2010. The calculated κ_{25} values were derived from the mass-balance model.

However, a comparison with an idealized model of complete retention of conductivity in the water body by the mass-balance model revealed that not all mass of electro-active substances came back into solution; numerically we found 53 %. The inflow of significant amounts of ion-rich groundwater was the proposed mechanism for the buffering of mixing processes during times of rising chemocline in Waldsee. A net outflow of groundwater during periods of chemocline erosion could contribute to the less pronounced increase of the measured monimolimnion conductivity in comparison to the model results, too.

In conclusion, iron meromixis as seen in Waldsee did not require two different sources of incoming waters, but the inflow of iron-rich deep groundwater and the aeration through the lake surface were sufficient for the formation and sustaining of permanent stratification.

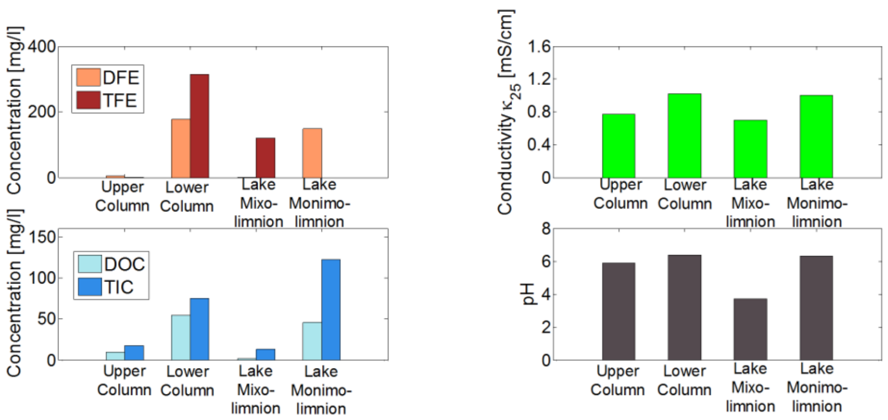

Figure 2.3: Water properties of samples from different water layers in Waldsee and the water column. (from Nixdorf and Boehrer, 2015)

3. Evaluating the reliability of time series analysis to estimate variable riparian travel times by numerical groundwater modelling

The content of this chapter is included in:

Nixdorf, E., Trauth, N., 2018. Evaluating the reliability of cross-correlation method to estimate riparian travel times under time variant hydraulic gradients. Hydrol. Process. 32 (3): 408-420.

The transition zones between rivers and adjacent riparian aquifers are locations of high biogeochemical activities that contribute to a removal of potentially hazardous substances in the aquatic system (Pinay et al., 2009; Zarnetske et al., 2012; Boano et al., 2014). Subsurface water travel times can be used as a proxy to evaluate the significance of these removal processes. Travel times of infiltrating river water from a river to a groundwater well can be determined by analysing fluctuations of natural tracers where contrasts between river water and groundwater are high, such as temperature (Anderson, 2005) and electrical conductivity (Sheets et al., 2002; Vogt et al., 2010; Schmidt et al., 2012). As an alternative, riparian travel times can be computed by using process-based numerical flow models (Trauth et al., 2013; Altenkirch et al., 2016).

In this study, it is demonstrated how alternating hydraulic gradients imposed by artificial and natural flood events influence travel times in the riparian zone and the limitation of approaches which calculate travel times based on analyzing EC time series are shown. For this purpose, travel times through the riparian aquifer of a slight meander loop at the Selke River in Germany were calculated.

The objectives of this study were:

1) Determine riparian travel times of infiltrating river water and their dynamics due to varying hydraulic conditions during storm events and phases of water mill operation
2) Evaluate the differences in resulting travel times between the EC time series analysis approach and the numerical particle tracking based on the groundwater flow model
3) Providing new inside in the transient mixing mechanism between river water and ambient groundwater in the riparian aquifer

Data loggers measuring hydrostatic pressure and EC with a temporal resolution of 10 min were installed in six monitoring wells along a transect on both sides of the riparian aquifer. EC values were internally corrected to values at the reference temperature 25°C. An additional data logger was placed at the riverbed. Travel times were analyzed by applying windowed cross-correlation on 16 EC-fluctuations induced artificially by an upstream water mill as well as by eight natural storm events occurring between September 2013 and February 2014:

$$\rho(k)=\frac{\sum_{i=1}^{n} EC_{River}(t_i)\cdot EC_{GW}(t_i+k)}{\sqrt{\sum_{i=1}^{n}(EC_{River}(t_i))^2\cdot\sum_{i=1}^{n}(EC_{GW}(t_i+k)^2}} \tag{2}$$

Where EC_{River} and EC_{GW} are the electrical conductivity [mS/cm] in river and groundwater at a time step t_i, ρ is the normalised correlation coefficient [-], n the total number of time steps and k the time lag. A two-dimensional numerical groundwater flow model was developed for the study area using the numerical code OpenGeoSys v5.7 (OGS) to simulate the transient behavior of the groundwater flow field during the investigation period. The study site was transformed in an unstructured mesh consisting of about 36 000 Elements.

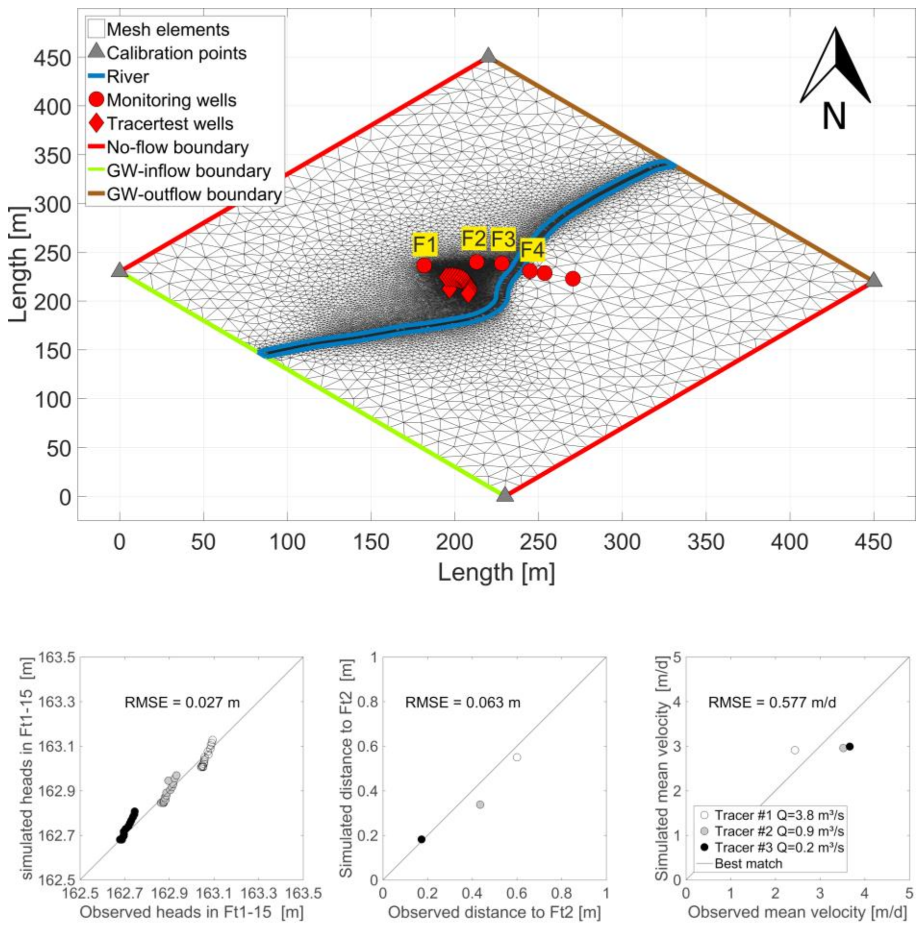

Figure 3.1: Description of the OGS groundwater flow model. Up: Configuration of the numerical groundwater flow model including the mesh. The location and names of the monitoring wells used for the EC time series analysis are labeled in yellow. Bottom: Calibration results of the groundwater flow model.

Hydraulic conductivity and porosity were assumed homogenous and isotropic. The coupling with the river was realized by assigning time-dependent head boundaries at the nodes representing the riverbed. The model was calibrated using the metrics derived from three salt tracer tests (Fig. 3.1) and the model-independent parameter estimation code PEST (Doherty, 2015). The calibrated groundwater flow model was applied together with a developed advective backward particle-tracking scheme to test the time-series analysis results on plausibility.

Although approaches based on EC time-series analysis have been applied and verified in many studies, possible limitations for the usage of EC fluctuation analysis were observed. The cross-correlation method produced only reasonable travel times for the artificial mill induced events. In contrast, cross-correlation analysis of the EC data during natural storm events resulted in unrealistically low travel times for the bulk of data sets (Fig. 3.2). Differences between the two estimation methods were up to two orders of magnitude. In addition, a decrease in EC was recorded earlier in the monitoring well F3 and F4 than the river for several events leading to physically implausible negative travel times.

Two effects could be delineated to be accountable for the disparities. Firstly, the low EC contrast between river and groundwater in connection with a strong damping of the infiltrating river EC signal into the subsurface during storm events. Secondly, old and less mineralized riparian water located between the river and the monitoring well produced bank-storage-driven EC breakthrough curves with earlier arrival times subsequently leading to the estimation of implausible riparian travel times (Fig. 3.3).

Event No.	F1	F2	F3	F4
	τ[h]	τ[h]	τ[h]	τ[h]
#1	-	18.8	-2.3	-1.5
#2	-	12.2	-1.8	-5.5
#3	1.8	41.3	-34.2	-5.8
#4	-	21.7	-3.2	2.2
#5	-	16.7	-15.5	-7.7
#6	-	1.5	24.2	5.2
#7	-	0.7	29.7	-11
#8	-	7.8	-5.8	1.2
Mean±std	1.8	15.1±13.1	2.8±2.1	0.63±0.3

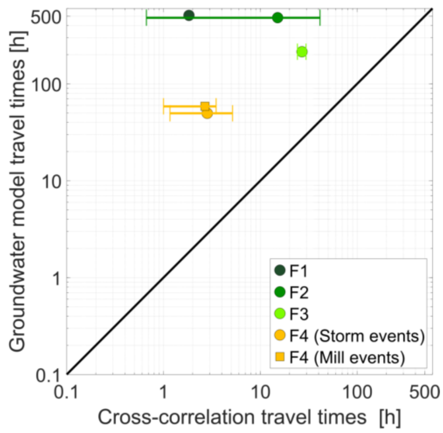

Figure 3.2: Comparison of estimated riparian travel times. Left: Travel times to each monitoring well for each storm event derived by EC time series analysis. Negative travel times were omitted for calculating the mean values. Right: Comparison of subsurface travel times estimated by the groundwater flow model and the cross-correlation analysis. The whiskers correspond to the spectrum of positive cross-correlation estimates.

By comparing the metrics of the storm event and mill event driven EC fluctuations, it is proposed that the applicability of EC time series datasets to estimate travel times can be roughly evaluated by analyzing the steepness of the rising river hydrograph and the corresponding declining chemograph. Additionally, the results of the study showed that in order to avoid misinterpreting the derived travel times, the origin of the EC signal in the riparian zone wells has to be known, which needs in turn detailed knowledge of the hydrology of the stream-groundwater interface.

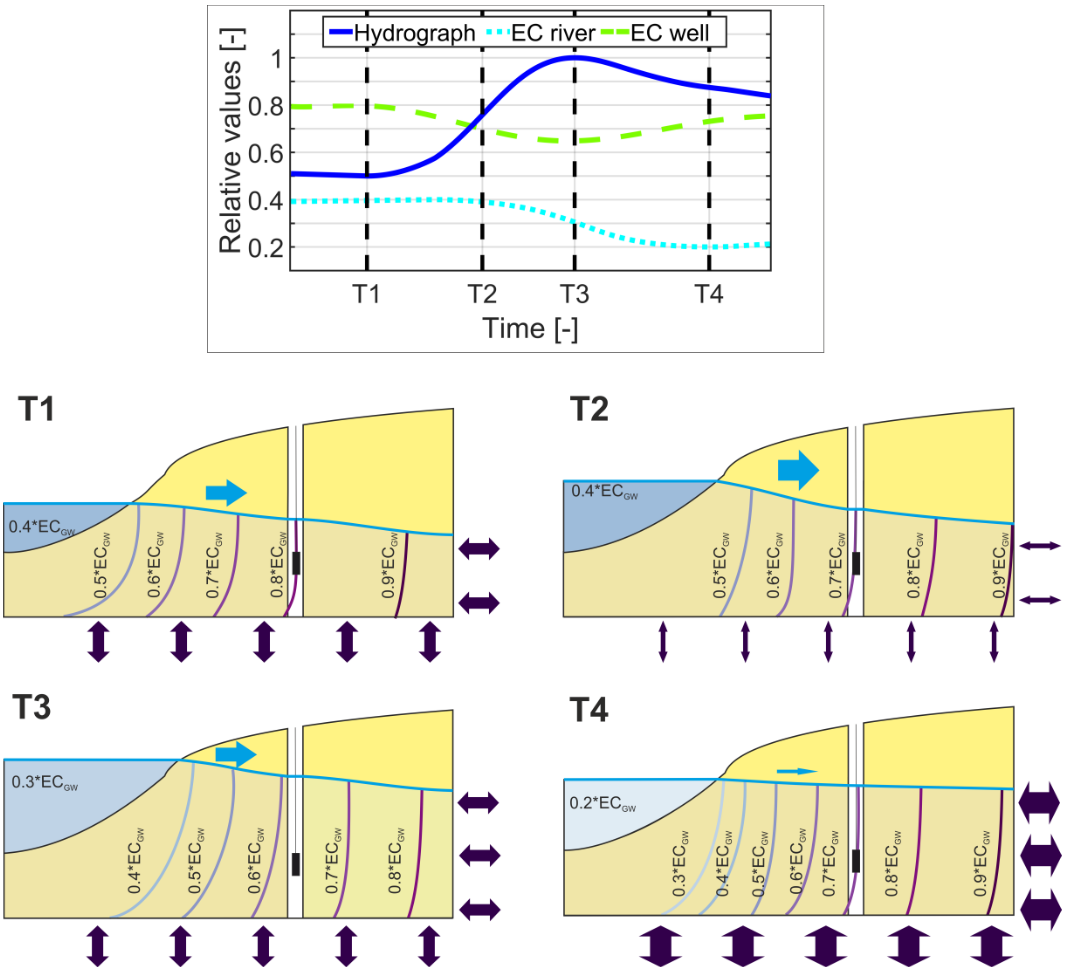

Figure 3.3: Conception of the development of bank-storage-driven EC breakthrough curves under losing conditions. The upper plot shows an idealized form of EC propagation during an event. The letters on the x-axis refer to the lower pictures in chronological order from time T1 to T4. The width of the dark purple double-arrows visualises the magnitude of ambient groundwater impact and the width of the horizontal light blue arrow indicates the magnitude of losing conditions. T1) EC distribution prior to an event. T2) The increasing river stage pushes low-EC riparian water into the monitoring well, but river EC remains constant. T3) At peak water level, river EC is declining but weakened hydraulic gradients are slowing the EC decrease in the monitoring well. T4) On the falling limb of the storm event, river EC reaches its minimum. However, weak losing conditions inhibit a further decline of EC in the monitoring well.

4. Multiscale groundwater contamination risk assessment in the Songhua River Basin

The content of this chapter is included in:

Nixdorf E, Chen C, Sun Y, Kolditz O. 2015. Persistent organic pollutants contaminate Chinese water resources: overview of the current status, challenges and European strategies. Environmental Earth Sciences 74 (2): 1837–1843

Nixdorf E, Sun Y, Lin M, Kolditz O. 2017. Regional assessment of groundwater contamination risk in the Songhua River Basin, China, by integrating public data sets, web services and numerical modelling techniques. Science of the Total Environment 605:598-609

Sachse A, **Nixdorf E**, Jang E, Rink K, Fischer T, Xi B, Beyer C, Bauer S, Walther M, Sun Y, et al. 2017. OpenGeoSys-Tutorial: Computational Hydrology II: Groundwater Quality Modeling. Springer.

Mao L, Danfeng J, Chifei C, Sun Y, Su J, Xi B, **Nixdorf E**. 2016. Groundwater Vulnerability Partition in Ashi River Basin. Research of Environmental Sciences 29 (12): 1773–1781 (in Chinese) DOI: 10.13198/j.issn.1001-6929.2016.06

In many regions of China, excessive exploitation and inappropriate activities at the land surface lead to and foster degradation of groundwater resources in many areas (Qiu, 2010; Jiang, 2009). Moreover, remediation of contaminated aquifers is cost intensive and time consuming and may not reach remedial objectives due to large storage, physical inaccessibility and retardation of contaminants (Travis and Doty, 1990). In this context, assessing the current and future groundwater contamination risk provides a useful tool to design and implement groundwater protection measures to prevent or reduce groundwater contamination (Zaporozec et al., 2002). Groundwater risk can be assessed by combining parameters of physical attributes using an index system (e.g. Aller et al., 1987). Although this approach is inexpensive and applicable on large scales, it is lacking a representation of physical processes in the subsurface (Rupert, 2001). Alternatively, process based approaches such as groundwater flow modelling allow to provide the most accurate representation of the interacting physical and chemical processes controlling groundwater contamination (Focazio et al., 2002) but need extensive field data and computational power (Butscher and Huggenberger, 2008), especially considering their application on larger scales (Ireson et al., 2006).

In this study, it is demonstrated how groundwater contamination risk can be evaluated by a combination of index and process-based assessment schemes in dependence of the spatial extension of the investigation area and the available data. The developed methodology was applied on Songhua River Basin in North-East China which surficial aquifers face threats of being polluted by numerous sources (Yang et al., 2010; Ma et al., 2013).
In this context, the objectives of this study were:

1. Compile data on existing individual contaminant investigations of rivers, lakes and aquifers in China
2. Develop a calibrated 3D groundwater flow and mass transport model for a process-based risk assessment of the groundwater relying water supply in an urban sub-catchment of Songhua River Basin
3. Assimilate data from public data sets, groundwater models as well as web service databases and integrate them in a framework to overcome constraints by input data scarcity for groundwater risk assessment of the entire Songhua River Basin
4. Provide maps of groundwater vulnerability, hazard potential and risk in Songhua River Basin at a high spatial resolution of 1 km² for usage by local environmental agencies

An extensive bibliographic study has been conducted to provide an overview about existing data on the pollution of Chinese water resources. Data on existing individual contaminant investigations of rivers, lakes and aquifers in China have been compiled for the largest river basins of China with focus on persistent organic pollutants. It could be shown that particularly for larger basins the amount of utilizable data on pollutant concentrations in natural waters in China is limited, which hinders the application of reactive-transport modelling schemes including complex reaction processes in the groundwater.
Subsequently, a three-dimensional groundwater flow model was developed for a smaller sub-catchment of Songhua River Basin representing the drinking water abstraction area of Acheng City with a population of about 500 000 people (Fig. 4.1). Based on a geological model obtained from drill log data and assuming a 1 m thick soil cover, a triangular finite element mesh with 9166 elements having a mean edge length of 500 m was set up using the Gmsh plugin (Geuzaine and Remacle, 2009) of the OpenGeoSyS DataExplorer (Rink et al., 2013). Subsequently, the three-dimensional transient groundwater flow model of the investigation area was set-up using the numerical code OpenGeoSys v5.7 (OGS). Dirichlet boundary

conditions were applied for the water level of Ashi River, which was assumed to decrease linearly northwards. Neumann boundary conditions were assigned on all nodes at the top of the model to map groundwater recharge. Groundwater abstraction was simulated by defining Neumann boundary conditions at the well positions in the main aquifer. All layers were treated as fully water-saturated. Hydraulic conductivities were determined by calibrating the stationary model with the current water levels in the abstraction wells and data from previous hydrogeological surveys.

A transient model run was designed assuming that the groundwater abstraction rate will increase by the factor 8 within 20 years due to economic growth and planned changes in the water supply system. Aside of changes in the flow field, the transport of pollutants in the groundwater emitting from four suspicious point sources (coal power plant, steel works, wood treatment facility and textile manufacturing facility) was simulated by the model. As chemical data were not available, the transport modelling was realized by solving the advection-dispersion equation using a conservative tracer with unity concentration, which constantly emitted from the top of the saturated zone:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (vc) \tag{4}$$

Where c is the concentration [ML^{-3}], v is the pore velocity vector [ML^{-1}], D is the hydrodynamic dispersion [L^2T^{-1}], t is time [T], ∇ is the gradient operator and $\nabla \cdot$ is the divergence operator.

The simulation showed that large changes of the pumping regime tremendously affect the flow field of the investigation area (Fig. 4-1). Initially, hydraulic gradients in the study area were in a range of one per thousand and groundwater velocities were less than 0.2 m/d. The main groundwater direction was from the headwaters in the south-west towards Ashi River. Under these conditions, the flow field was affected by the water abstraction only very locally in the northern part of the well field where the well density is highest. In contrast, the groundwater model could show that an increase of abstraction lead to an increase of groundwater velocities up to 0.7 m/d, particularly near the wellfields. Groundwater levels decreased more than 10 meters in the northern well field, which probably has a significant effect on the groundwater dependent parts of the ecosystem.

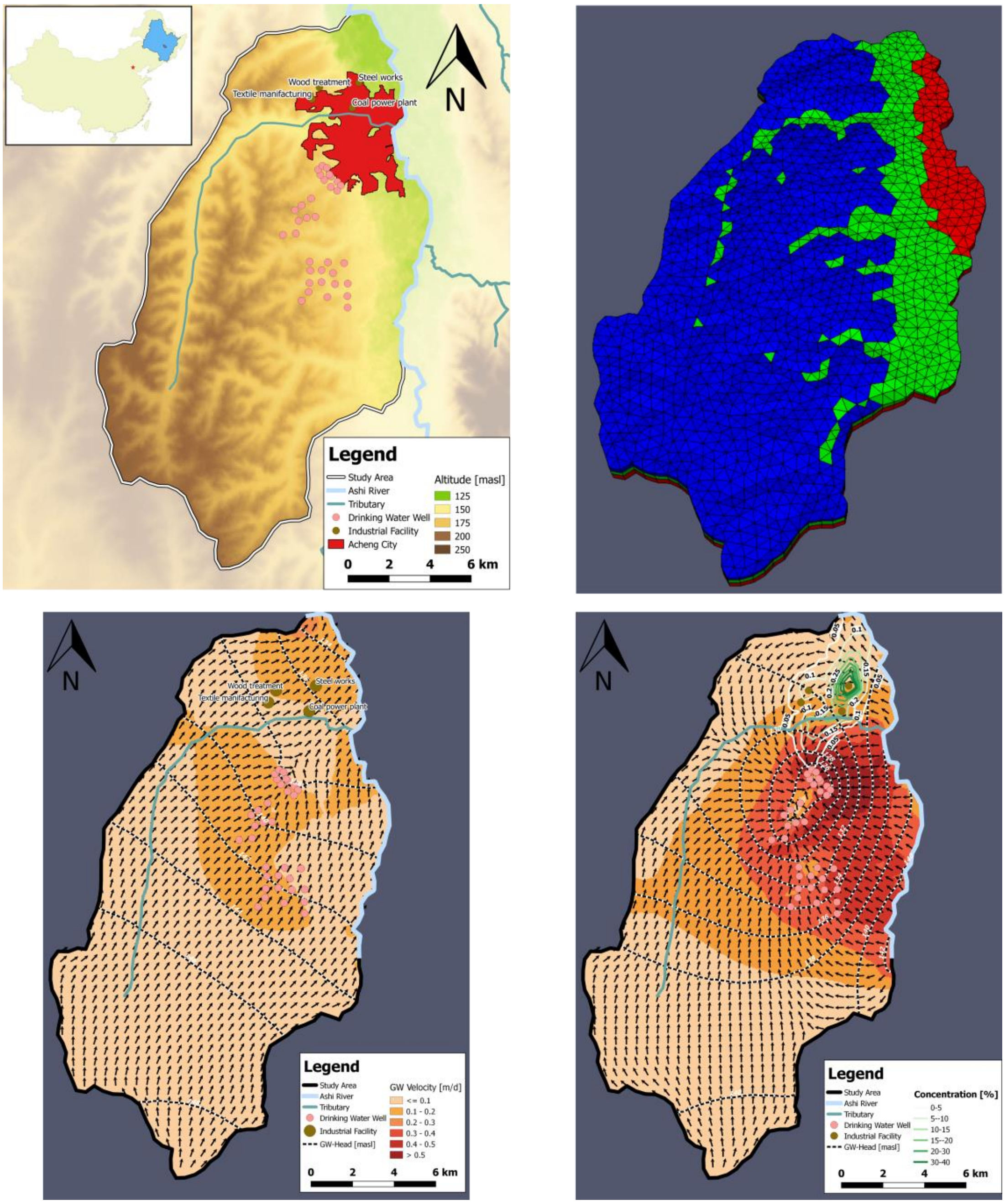

Figure 4.1: Numerical flow and matter transport model of the Acheng study area. Top-left: Location of suspicious sites and abstraction wells in the study area. The map at the upper left corner shows the location of Ashi River Basin within the Songhua River Basin (blue area) in China. Top-right: Mesh of the model domain consisting of the surficial aquifer (blue color), the aquitard (green color) and the main aquifer (red color). Bottom-left: Groundwater flow field indicated by black arrows at the beginning of the simulation. The groundwater velocities were calculated for the main aquifer and in planar direction. Bottom-right: Groundwater flow field and distribution of relative pollutant concentration in the main aquifer after 20 years of simulation.

Additionally, reversed groundwater flow directions in the northern and eastern part of the study area lead to the transfer of groundwater from the industrial areas of Acheng city towards the water abstraction wells. Quantitatively, the 5 % isoconcentration line reached the northern edge of the wellfield within simulation time. The major aquifer below the steel works could be identified to be the most vulnerable zone due to its less protection by upper subsurface layers. Chemical degradation and transport processes in the partially saturated subsurface tend to delay the spreading for pollutants in the subsurface. Since the numerical transport model did not include these effects, derived isoconcentration lines can be seen as a conservative estimate. However, due to the long tradition of heavy industry in the study area, additional pollution plumes in the groundwater might exist which could put an additional threat to the water supply system due to the proposed change of groundwater directions. Hence, the study revealed that additional hydrogeological and hydrogeochemical measurements are needed in combination with a more profound hazard assessment for the northern part of the study area before conducting significant changes of the pumping regime in the wellfields.

For the large scale of Songhua River Basin, groundwater risk was identified using an index assessment system by combining the DRASTIC method (Aller et al., 1987) for groundwater vulnerability assessment and a hazard assessment method based on land cover and a hazard inventory of point pollution sources (Fig. 4.2). A GIS platform was used to scale and overlay input datasets from different sources and to compute and visualize evaluation results in a spatial grid resolution of 30 arcsec (~ 1km^2).

To overcome data limitations on the large scale, a framework was developed which integrated data from public datasets, web services and numerical modelling techniques into the groundwater risk assessment (Fig. 4.2). The majority of parameters for the risk index assessment were calculated based on geospatial data sets obtained from national agencies and international organizations.

For the depth to groundwater calculation, a 2D stationary groundwater flow model of Songhua River Basin was set up using OpenGeoSyS. In contrast to conventional interpolation schemes, the groundwater flow model allowed to include the impact of groundwater recharge, abstraction rates and the watercourse of the major rivers on the distribution of drawdowns in the Songhua basin. The groundwater flow model, which consists of about 130000 finite elements, was calibrated using the yearly average of hydraulic heads measured in 59 monitoring wells. Although information about the dominant hydrogeological structures was available, the calibration process showed that a heterogeneous setting only slightly improved the calibration result but tremendously increased model equifinality. Hence, model subsurface properties were treated as homogeneous and isotropic (Fig. 4.3).

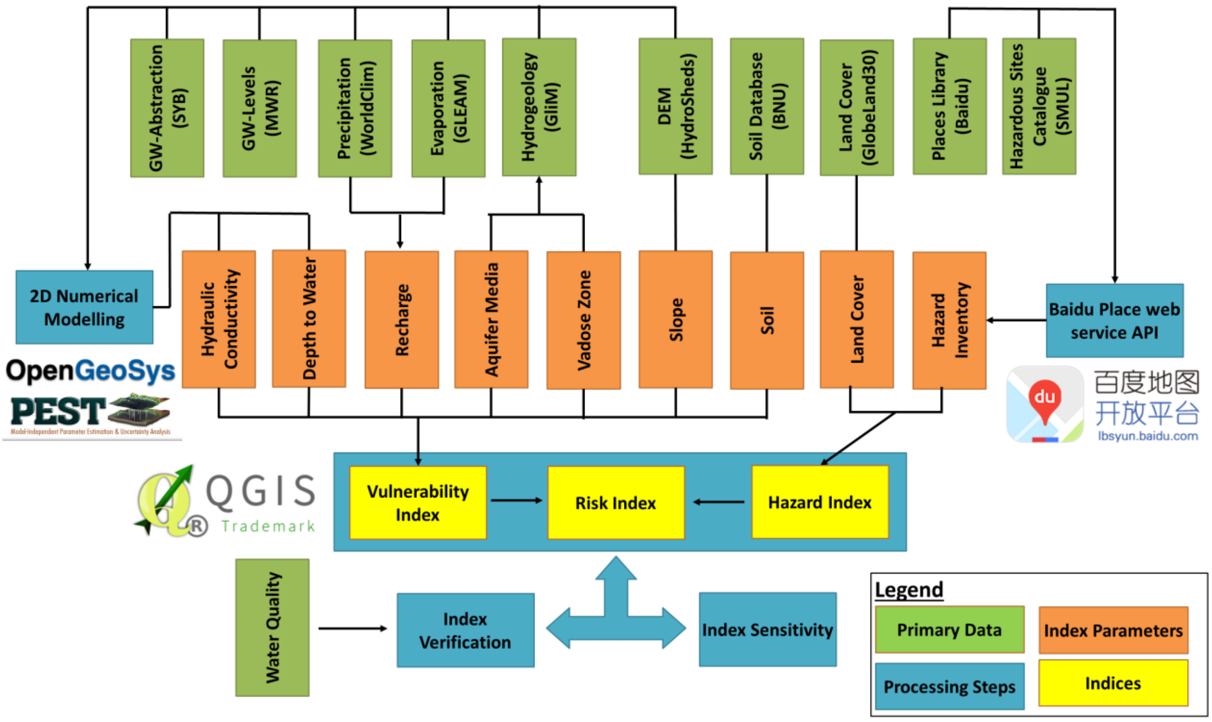

Figure 4.2: Schematic flowchart of the methodology adopted for this study. The brackets in the green boxed indicate the data sources. (from Nixdorf et al., 2017)

For the establishment of a hazard inventory, information on potentially hazardous sites were queried from a web service database using the place web service API of Baidu Maps (Baidu Inc., 2016). The Baidu Place API allows up to 2000 requests per day and provides a maximum of 20 results per request. Songhua River Basin was delineated into 94 cells with a cell size of 1° applied for each data request. The request procedure was automatized by using a Python script in a way that if 20 results were received by a request, the affected geographical boundary cell was quartered and four new requests were started. If necessary, this procedure was repeated until the desired final cell resolution of 30 arcseconds was reached. Finally, all results were processed and assigned with the corresponding hazard class ratings from a German hazard rating system (SMUL, 1997).

The application of this methodology to the entire Songhua River Basin demonstrated that vulnerability and harmfulness of a significant part of the catchment's plain areas was emphasized (Fig. 4.4). Correlation analysis further revealed a strong tendency that a higher vulnerability index value was associated with a higher hazard index value. Summarizing, about 1% of Songhua River Basin consist of areas with high or very high contamination risk, mainly located in the vast plain areas with hotspots particularly in the Changchun metropolitan area.

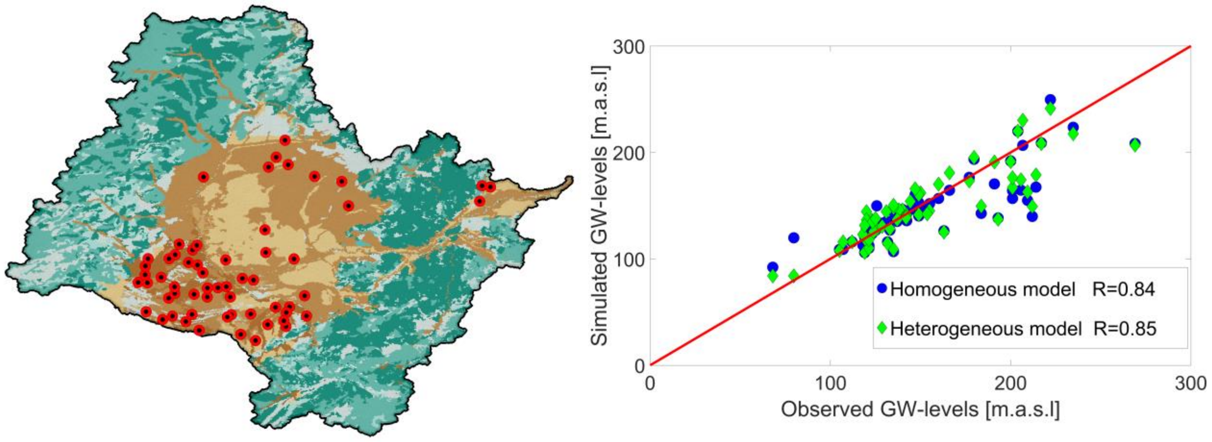

Figure 4.3: Mesh structure and calibration results of the groundwater model. Left: 2D model domain colored by the different hydrogeological layers. Red dots show the well locations. Right: Observed and measured groundwater wells for the stationary calibration set-ups. (from Nixdorf et al., 2017)

Additional smaller scattered areas associated with high and highest risk to be polluted are located in the urban areas around the cities of Baicheng and Songyuan in the southeastern part of the catchment. Low groundwater risks were obtained for the mountainous headwaters of Songhua River mainly due to less potential hazards and favorable vulnerability conditions such as steep slopes and low hydraulic permeabilities.

Sensitivity analysis could show that groundwater levels and pollution point sources play a significantly larger impact in assessing areas with a high risk of being polluted than originally assumed by the index scheme. This highlights the importance of using process-based flow models and comprehensive web databases to improve parameter estimation.

Despite limitations in resolution and input data consistency, the derived groundwater vulnerability, potential hazard and groundwater contamination risk maps support decision-making in the field of future land planning and groundwater management and will aid avoiding future contamination of the groundwater by considering the vulnerability of an area before high-risk activities are allowed to take place. The usage of open source software and datasets accessible to public ensure that the methods of this study are highly reproducible in other areas of China and even worldwide. Although subjectivity was unavoidable in the study, some measures, such as the aggregation and classification of different factors in a unified form, could overcome this disadvantage to some extent. Further efforts should be conducted to overcome present resolution limitations in order to make the maps more useful on a local scale and to improve validation concepts. Future studies should include the temporal changes of groundwater contamination risk in the area, e.g. due to the man-made lowering of the groundwater table or climate change impacts to predict short-term effects of land-planning decisions.

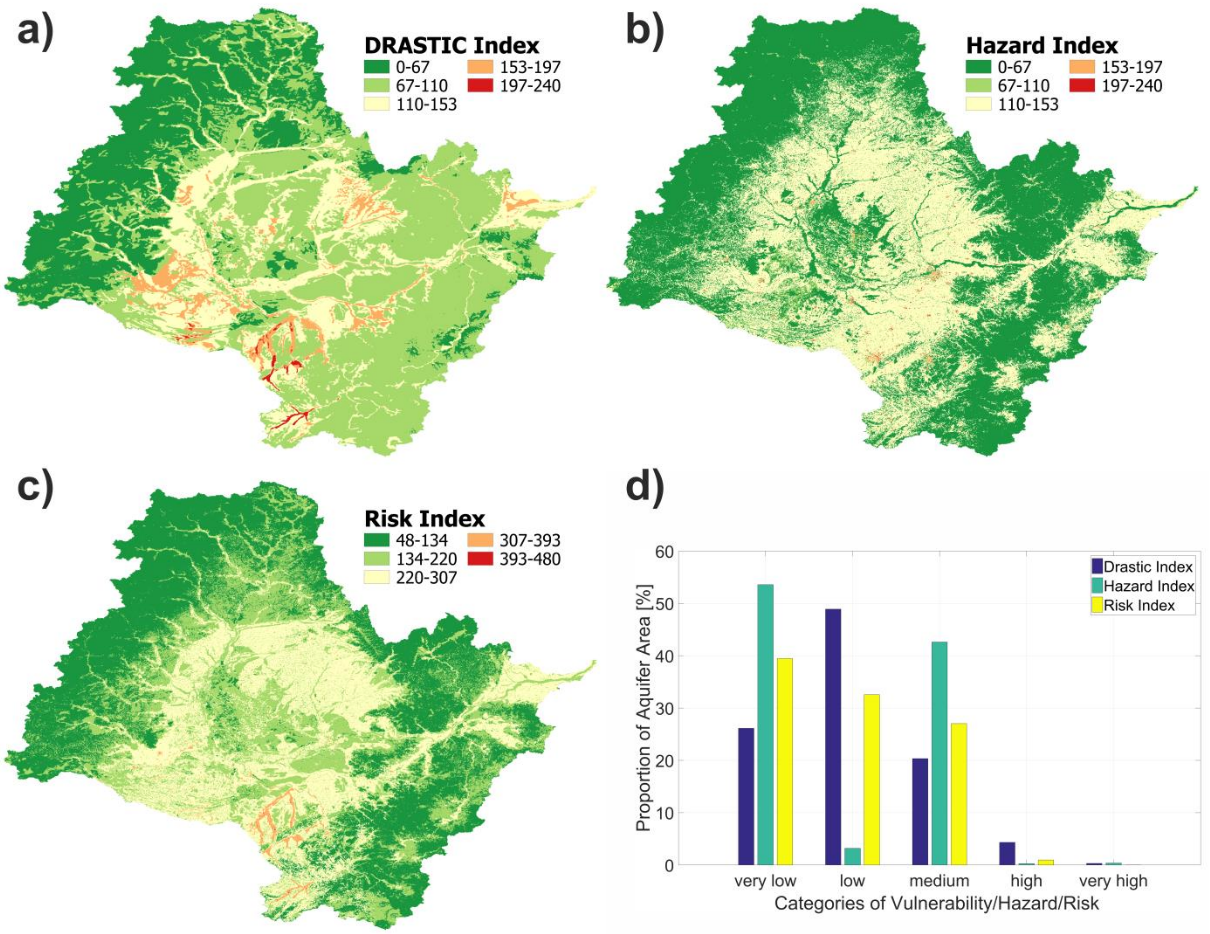

Figure 4.4: Groundwater index maps of Songhua River Basin. DRASTIC vulnerability index(a), hazard index (b) and risk index (c) were classified in five categories from very low (dark green color) to very high (red color) groundwater vulnerability, potential harmfulness and pollution risk. The percentage frequency distribution of all index map categories is given by (d) (from Nixdorf et al., 2017).

5. Summary

5.1 Main achievements

This thesis combines several approaches and applications for investigating flow dynamics in groundwater-dependent water systems on different scales, including the development of numerical modelling schemes for different purposes with a close interlinkage to simultaneously conducted field measurements and data acquired from multiple data sources. The focus of the thesis was to use this combination of approaches to develop tailor-made solutions addressing practical problems in the investigated study areas. The key achievements are listed comprehensively in the following:

1.) In a German mining lake with a permanent induced stratification, the seasonal dynamics of electro-active species could be quantified by processing a long-term dataset of vertical EC-profiles using a 1D layered model of the stratified lake. In addition, a column experiment was set-up to verify the proposed biogeochemical reaction system in the lake.

2.) A mathematical mass balance model of the lake was developed to reveal the impact of internal substance transport, mixing processes and groundwater inflow on the stability of the lake meromixis. The high importance of exchange fluxes between the groundwater and the lake could be demonstrated.

3.) A numerical groundwater flow model, comprising the riparian aquifer along a meander of the Selke River, was set up and successfully calibrated under transient conditions using the travel times estimated from three independent salt tracer tests. Using the RMSE metric, calibration results showed high agreement with the measurements.

4.) The groundwater model was successfully combined with an advective backward-in-time numerical particle tracking approach to prove the riparian travel times obtained by the analysis of propagating EC time series during storms and induced events. Subsequently, possible limitations of the applicability of the latter approach for storm events was demonstrated and new inside in the transient mixing mechanism between river water and ambient groundwater in the riparian aquifer under time variant hydraulic gradients was provided.

5.) The contamination of rivers, lakes and aquifers in China with organic contaminants was documented by a comprehensive bibliometric study. It could be shown that the availability of comprehensive data is rare, particularly with regard to groundwater quality.

6.) A three-dimensional groundwater flow and mass transport model was developed and calibrated for an urban sub-catchment area of Songhua River Basin in China. The model was utilized to prove that the proposed increase of groundwater abstraction rates will significantly change flow velocities and directions and may lead to the inflow of potentially contaminated groundwater from industrial areas into the water supply system.

7.) A novel method for integrating data from public data sets, groundwater models as well as web service databases in an index scheme for the groundwater risk assessment of large river basins was developed for the Songhua River Basin. In particular, it could be proved that using data queries from web service database in combination with a hazard classification system to delineate potential pollution sources provides an appropriate alternative to cadastral data if access to the latter ones is restricted.

8.) A geographic information system was utilized to provide maps classifying groundwater vulnerability, hazard potential and risk in the entire Songhua Basin at a high spatial resolution of 1 km^2 which allows future usage by local environmental agencies.

5.2 Conclusions

The presented doctoral thesis emphasizes the importance of combining numerical modelling approaches with field measurements and other traditional (public datasets) and emerging (e.g. web service databases) data sources to investigate hydrological processes in groundwater dependent water systems. A future question is how the individual parts of the doctoral thesis can be integrated to a more holistic approach to address issues on the basin scale. Although the hydrological system shown in Fig. 1.2 belongs to a fictional basin, it visualizes the important fact that the majority of basins in the world are subject to diverse pressures and challenges for both, water quantity and water quality, including all the processes covered by this doctoral thesis and beyond. Hence, for responsibly addressing these issues on a basin scale, a broader understanding of process relevance is needed for which the results of this doctoral thesis can be used.

An excellent real-case example covering all the interaction processes investigated in this thesis is Poyang Lake, which is, by maximum annual extension, the largest freshwater lake in China. Although being in better hydrological conditions than many other large lakes in China (Ministry of Environmental Protection, 2017), its water quality is continuously deteriorating due to pollution pressures from agricultural, mining and industrial sources as well as due to water budget changes caused by hydraulic construction measures and changing climate conditions (Duan et al., 2016; He et al., 1998; Xu and Wang, 2016).

The seasonal water level change of Poyang Lake of up to 10 m propels very dynamic interaction processes with the surrounding groundwater. In winter, low water levels result in a river-like system behavior of Poyang Lake. Despite the fact that 77 % of the run-off to Poyang Lake is formed by base flow from shallow groundwater (Hu et al., 2013), the role of the widely fluctuating groundwater-surface water interface on determining the water quality and quantity in Poyang Lake is not investigated yet (Li et al., 2016). This research gap can be filled on a small and medium scale by extending the measurement and numerical modelling methodology developed in chapter 3 of the thesis. Considering the size of Poyang Lake, combined approaches of using remote sensing data and open web databases together with simple but effective large-scale models as developed within chapter 4 of this thesis may be extended and implemented on Poyang Lake to evaluate the threats on the shallow groundwater and the lake. In addition, simple mass-balance approaches as shown in chapter 2 of the thesis may be beneficial to upscale and quantify the impact of estimated groundwater-surface water and matter exchange fluxes on the lake scale.

However, much demanding work needs to be done in order to apply the developed assessment approaches for investigating groundwater dependent problems on the large basin scale:

1.) It is necessary to develop coupling strategies of processes inside and between the water compartments, which should be simple but efficient in dependence on the spatial-temporal scale of the investigation. In this thesis, the coupling of connected water compartments was simplified to boundary conditions and matter transport was in most cases considered as purely advective or reduced to mass-budget calculations. These approaches are efficient in terms of computation but are lacking feedback between both systems (Furman, 2008). In case of Poyang Lake, an efficient coupling between numerical groundwater flow models and models representing the surface water body is required in order to minimize the amount of numerical intervention necessary for simulating the impact of a changing inundation depth on the model and to represent the dynamic hydro-chemical boundary conditions of the hydrological system.
2.) A joint framework is needed to develop hydrological concepts of a study area collectively by modelers and experimentalists (Weiler and McDonnell, 2004). Using the proposed example of Poyang Lake, numerical models should, beside of their ability of scale extrapolation, explore the role and significance of single parameters on the forces determining fluid and solute fluxes in order to design exploration and measurement campaigns in the field and subsequently benefit from them and vice versa.
3.) The on-the-fly integration of data into the modelling framework and scientific visualization methods for different degrees of complexity will be essential further steps to accelerate data analysis, to forecast changes in the hydrological system as soon as possible, to delineate the existence of data gaps and to facilitate the communication e.g. between modelers and experimentalists. A promising example is the environmental information system developed for Lake Chao in China, which combines, organizes, updates and visualizes data from different numerical models and monitoring stations (Rink et al., 2017).

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Appendix

A1. Soft copy content

The soft copy content of the dissertation is provided on a digital medium attached to the paper version of this dissertation. In addition, the supplementary material is accessible as a compressed ZIP file labeled “Supplementary_Material.zip” at the Microsoft OneDrive file hosting service using the following link:

https://1drv.ms/u/s!AmP4zB6nWjfpilzAPzEbEfNJsOGd

A list of the soft copy content as well as a description of each dataset is given by Tab. A1.

Table A1: Structure of the digital appendix

Chapter path	Subdirectory path	Folder name	Description
.\Chapter2\	\Measurements\	\Column\	Raw time series measured by the data logger during the column experiment
		\Lab_Analysis\	Laboratory analysis of the samples taken at the end of the column experiment
		\Lake_Waldsee\	Raw time series data measured by different types of data loggers during the monthly profiling of Lake Waldsee. The file “Waldsee_ bathymetry.txt” contains the bathymetry of Lake Waldsee
	\Mixing_Model\	-	Calculations of monthly mass-balances provided as Microsoft excel spreadsheet
	\Scripts\	\Conversion\	MATLAB scripts to convert the raw data of each data logger type to a unified format
		\Processing\	MATLAB scripts to calculate derived parameters such as summed conductivity and to plot the results

.\Chapter3\	\GW_Model\	\Calibration\	OGS input files and PEST input files to set up and calibrate the groundwater flow model of the riparian zone during the period of the salt tracer tests. Additionally, results summary and MATLAB scripts for postprocessing are provided
		\Comparison \	OGS input files for the groundwater model simulating the period of the storm events. Additional MATLAB scripts to process the derived riparian travel times
		\Particle_Tracker\	Numerical advective particle tracker written in MATLAB
		\Raw_Data\	Collection of hydrological, topographical and chemical data used for model set-up and calibration
	\Time_Series\	\Peak_Picking\	Peak picking algorithm for the cross-correlation function written in MATLAB
.\Chapter4\	\GW_Model\	\Ashi_Subbasin\	OGS input files for the transient groundwater and mass transport simulation of Ashi River Subbasin
		\Songhuajiang\	OGS Input files for the stationary groundwater simulation of Songhua River Basin with either homogeneous or heterogeneous hydrogeological setting
	\Point_Hazards\	\Input_Files\	Chinese translations of facility included in the German hazard rating system. Grid cells of the search grid covering Songhua River Basin
		\Processing\	Python script which allows to send a

			search query for point hazards to the Baidu Maps API and retrieve, process and save results
		\Output\	Results of the search query for point hazards in Songhua River Basin
	\Risk_Maps\	\Parameter\	Geotiff raster files including all parameters required for the calculation of the vulnerability, hazard and risk indices
		\Scripts\	MATLAB scripts to compute the indices by using defined weighting schemes provided as *.txt files
		\Sensitivity\	MATLAB scripts to calculate sensitivity and statistics of the derived index raster datasets

A2. Publications

A2.1 Nixdorf et al. (2015)

Title: Persistent organic pollutants contaminate Chinese water resources: overview of the current status, challenges and European strategies

Authors: Erik Nixdorf, Cui Chen, Yuanyuan Sun, Olaf Kolditz

Abstract: In order to get a better overview of the national scale of POP-related water pollution in China, the EU-China Environmental Sustainability Programme of the European Union and the international Helmholtz network, RCEIS, are supporting the enormous task of compiling data on existing individual contaminant investigations of rivers, lakes and aquifers in China. The differences regarding POP contamination in the water body status evaluation schemes of China and the EU become evident as the authors point out a selection of European case studies of POP-contaminated water resource assessments and successful remediation strategies. An ongoing cooperation project between China and the EU is introduced to show exemplarily that the adoption of existing strategies will offer huge potential opportunities for China to manage its water quality challenges and to enhance the existing scientific cooperation between China and the EU.

Full reference: Nixdorf E, Chen C, Sun Y, Kolditz O. 2015. Persistent organic pollutants contaminate Chinese water resources: overview of the current status, challenges and European strategies. Environmental Earth Sciences 74 (2): 1837–1843 DOI: 10.1007/s12665-015-4448-x

A2.2 Nixdorf & Boehrer (2015)

Title: Quantitative analysis of biogeochemically controlled density stratification in an iron-meromictic lake

Authors: Erik Nixdorf, Bertram Boehrer

Abstract: Lake stratification controls the cycling of dissolved matter within the water body. This is of particular interest in the case of meromictic lakes, where permanent density stratification of the deep water limits vertical transport, and a chemically different (reducing) milieu can be established. As a consequence, the geochemical setting and the mixing regime of a lake can stabilize each other mutually. We attempt a quantitative approach to the contribution of chemical reactions sustaining the density stratification. As an example, we chose the prominent case of iron meromixis in Waldsee near Doebern, a small lake that originated from near-surface underground mining of lignite. From a data set covering 4 years of monthly measured electrical conductivity profiles, we calculated summed conductivity as a quantitative variable reflecting the amount of electro-active substances in the entire lake. Seasonal variations followed the changing of the chemocline height. Coinciding changes of electrical conductivities in the monimolimnion indicated that a considerable share of substances, precipitated by the advancing oxygenated epilimnion, re-dissolved in the remaining anoxic deep waters and contributed considerably to the density stratification. In addition, we designed a lab experiment, in which we removed iron compounds and organic material from monimolimnetic waters by introducing air bubbles. Precipitates could be identified by visual inspection. Eventually, the remaining solutes in the aerated water layer looked similar to mixolimnetic Waldsee water. Due to its reduced concentration of solutes, this water became less dense and remained floating on nearly unchanged monimolimnetic water. In conclusion, iron meromixis as seen in Waldsee did not require two different sources of incoming waters, but the inflow of iron-rich deep groundwater and the aeration through the lake surface were fully sufficient for the formation of iron meromixis.

Full reference: Nixdorf E, Boehrer B. 2015. Quantitative analysis of biogeochemically controlled density stratification in an iron-meromictic lake. Hydrology and Earth System Sciences 19 (11): 4505–4515 DOI: 10.5194/hess-19-4505-2015

A2.3 Nixdorf et al. (2017)

Title: Development and application of a novel method for regional assessment of groundwater contamination risk in the Songhua River Basin

Authors: Erik Nixdorf, Yuanyuan Sun, Mao Lin, Olaf Kolditz

Abstract: The main objective of this study is to quantify the groundwater contamination risk of Songhua River Basin by applying a novel approach of integrating public datasets, web services and numerical modelling techniques. To our knowledge, this study is the first to establish groundwater risk maps for the entire Songhua River Basin, one of the largest and most contamination-endangered river basins in China. Index-based groundwater risk maps were created with GIS tools at a spatial resolution of 30arc sec by combining the results of groundwater vulnerability and hazard assessment. Groundwater vulnerability was evaluated using the DRASTIC index method based on public datasets at the highest available resolution in combination with numerical groundwater modelling. As a novel approach to overcome data scarcity at large scales, a web mapping service based data query was applied to obtain an inventory for potential hazardous sites within the basin. The groundwater risk assessment demonstrated that <1% of Songhua River Basin is at high or very high contamination risk. These areas were mainly located in the vast plain areas with hotspots particularly in the Changchun metropolitan area. Moreover, groundwater levels and pollution point sources were found to play a significantly larger impact in assessing these areas than originally assumed by the index scheme. Moderate contamination risk was assigned to 27% of the aquifers, predominantly associated with less densely populated agricultural areas. However, the majority of aquifer area in the sparsely populated mountain ranges displayed low groundwater contamination risk. Sensitivity analysis demonstrated that this novel method is valid for regional assessments of groundwater contamination risk. Despite limitations in resolution and input data consistency, the obtained groundwater contamination risk maps will be beneficial for regional and local decision-making processes with regard to groundwater protection measures, particularly if other data availability is limited.

Full reference: Nixdorf E, Sun Y, Lin M, Kolditz O. 2017. Regional assessment of groundwater contamination risk in the Songhua River Basin, China, by integrating public data sets, web services and numerical modelling techniques. Science of the Total Environment 605:598-609 DOI: 10.1016/j.scitotenv.2017.06.126

A2.4 Nixdorf & Trauth (2018)

Title: Evaluating the reliability of time series analysis to estimate variable riparian travel times by numerical groundwater modelling

Authors: Erik Nixdorf, Nico Trauth

Abstract: The transition zones between rivers and adjacent riparian aquifers are locations of high biogeochemical activities that contribute to a removal of potentially hazardous substances in the aquatic system. The potential of the removal processes depends on subsurface water travel times, which can be determined by using the propagation of electrical conductivity (EC) signal from the river into the riparian aquifer. Although this method has been applied and verified in many studies, we observe possible limitations for the usage of EC fluctuation analysis. Our findings are based on EC time-series analyses during storm events and artificial hydropeaks induced by watermill operations. Travel times derived by cross-correlation analysis were compared with travel times calculated based on backward particle tracking of a calibrated transient numerical groundwater flow model. The cross-correlation method produced only reasonable travel times for the artificial hydropeaks. In contrast, cross-correlation analysis of the EC data during natural storm events resulted in implausibly negative or unrealistically low travel times for the bulk of the data sets. We conclude that the reason for this behaviour is, firstly, the low EC contrast between river and groundwater in connection with a strong damping of the infiltrating river EC signal into the subsurface during storm events. Secondly, the existence of old and less mineralized riparian water between the river and the monitoring well resulted in bank-storage-driven EC breakthrough curves with earlier arrival times and the subsequent estimation of implausible riparian travel times.

Full reference: Nixdorf, E., Trauth, N., 2018. Evaluating the reliability of cross-correlation method to estimate riparian travel times under time variant hydraulic gradients. Hydrol. Process. 32 (3): 408-420 DOI: 10.1002/hyp.11428