An integrated study of hydraulic anisotropy and its impact on saltwater intrusion in an inland aquifer: Laboratory method, modeling, and recommendations

Dissertation

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老子曰:"上善若水,水善利万物而不争"。《道德经•道经》第八章,公元前六世纪

Laozi said,

The best virtue is like that of water,
which benefits everything in the world,
but never contends its own contribution.

Chapter 8, Tao Ching, Tao Te Ching, 6th century BC

Preface

The present thesis was conducted as my doctoral work within the Erasmus Mundus External Cooperation Window (EM ECW) Programme (Project Lund, Lot 14a – China) at Freie Universität Berlin. The work outlined in this thesis was carried out over a period of four years (September 2010 to August 2014). Financial support was provided by the EM ECW (September 2010 to June 2013).

The core chapters of this thesis have been published or submitted for publication, to which I contributed as the first author. I have been in charge of the development and conduction of the research work described. I have been responsible for the scientific content and the preparation of manuscripts, including literature review, data interpretation, preparation of figures and tables, and manuscript writing. Co-authors have mainly played an advisory and supervisory role.

The thesis contains the contributions by Dr. Thomas Taute, Christian Menz, Ulrike Maiwald, Dr. Miaomiao Ma as well as the technicians of the pigadi GmbH and the Berliner Wasserbetriebe (BWB) for field sampling.

Declaration of originality

I hereby certify, as the author of this thesis, and as one of the main authors of the publications arising, that I was the person involved in fieldwork, organization, implementation, analysis, evaluation, and manuscript preparation.

I declare that this thesis and the work reported herein is to the best of my knowledge, except as acknowledged in the text, and that the work was not submitted previously to any other institution.

Jialiang Cai

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This long journey of my doctoral work is eventually coming to the end. At this very moment, I would like to express the greatest and deepest gratitude to my supervisors, co-advisors, colleagues, friends as well as my family. Without your numerous help, support, and company, it definitely would not be possible for me to accomplish such a challenge.

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Last but not least, I would like to express the most earnest gratitude to my parents, Jinlong Cai and Peiping Chen, along with other family members, for unconditionally loving und supporting me in all my pursuits.

Summary

The two-dimensional hydraulic anisotropy (a), defined as the ratio of horizontal to vertical hydraulic conductivity (K_h/K_v), is a standard parameter of hydrogeological characterization, However, a is not routinely determined and correspondingly its value is often empirically set to 10 in the numerical modeling studies for solving anisotropic problems in sediments, owing to the fact that one of the challenging tasks hydrogeologists face today is the high-resolution characterization of directional hydraulic conductivity (DHC) in sediments. Therefore, an integrated laboratory method, called modified constant-head permeameter test (MCHPT), was established for the efficient determination and verification of consistent DHC values in fine-to-medium sandy sediments, based on a new methodological framework that includes a precise and standardized procedure for preparing the experimental setup.

As known, detailed information on a can provide an important fundament for modeling transport phenomena in sediments, e.g. saltwater intrusion. Saltwater intrusion is a widespread problem of continuing great practical interest in many coastal and inland aquifers all over the world, which is considered a special category of contamination to make groundwater unsuitable for human, industry and irrigation uses. There is an increasingly significant effect of salinization in most abstraction wells with a great depth of ~ 50 m below the surface in an inland aguifer at the Beelitzhof waterworks in southwestern Berlin (Germany) and a very thin film of saline groundwater (centimeter scale) has been observed in fine-to-medium sandy sediments on the top of the Rupelian clay at the site, thus, it could be assumed that Elsterian glacial channels would be in the close vicinity of the site, which results in saltwater upconing owing to pressure release by pumping a large amount of groundwater in drinking-water-production wells. Consequently, the impact of a on the intensity of saltwater intrusion due to pumping at the site was demonstrated based on the precise quantification of an a value of 2.3 using MCHPT in comparison with the empirical value of 10, by developing a conceptual model representative of the field situation and implementing it in a numerical density-dependent groundwater flow and solute transport model.

During the aforementioned modeling study, it has been found to be not yet able to be proven at the site whether there are hydraulic windows in the clay caused by glacial erosion or not. Therefore, two hypotheses about geological conditions in an inland aquifer leading to pathways for upwelling deep saline groundwater due to pumping, were raised as to: (1) there are windows in the clay, where their locations are uncertain; and (2) there are no windows in the clay, but the clay is partially thinned out but not completely removed by glacial erosion, so salt can merely come through the clay upwards by diffusion and eventually accumulate on its top. These hypotheses were tested to demonstrate the impact of the lateral distance between windows in the clay and the well, as well as salt diffusion through the clay depending on its thickness on saltwater intrusion in the pumping well respectively. Hypothesis 1 was validated with 4 scenarios that windows could occur in the clay at the site and their locations under some conditions could significantly cause saltwater intrusion, while hypothesis 2 could be excluded, because salt diffusion through the clay with thickness greater than 1 m at the site was not able to cause saltwater intrusion.

On the basis of the validated deep saline-groundwater source, two recommendations of pumping optimization were provided to control saltwater intrusion in an inland aquifer for drinking-water supply at the site. In terms of pumping-rate reduction, the optimal pumping rate was validated for eliminating the effect of saltwater intrusion. Its value could be set 1.39×10^{-2} m³/s (50 m³/h) or 5.56×10^{-3} m³/s (20 m³/h), if the requirement of drinking water palatability were good or excellent, respectively. With regard to pumping-pattern rearrangement, the well construction was modified to access bank filtration for eliminating the effect of saltwater intrusion.

Overall, this thesis has conducted an integrated study of hydraulic anisotropy and its impact on saltwater intrusion in an inland aquifer. Its highlights can be summarized as to: (1) It is the first time to efficiently determine and verify precise consistent DHC values in fine-to-medium sandy sediments by developing an integrated laboratory method called MCHPT; and (2) it is the first time to identify deep saline-groundwater sources in an inland aquifer and validate their impacts on saltwater intrusion by testing for two hypotheses about geological conditions leading to pathways for upwelling deep saline groundwater due to pumping, using a density-dependent groundwater flow and solute transport model.

Zusammenfassung

Die zweidimensionale hydraulische Anisotropie (a), die als das Verhältnis der horizontalen zur vertikalen hydraulischen Leitfähigkeit (K_h/K_v) definiert ist, ist ein Standardparameter der hydrogeologischen Charakterisierung und stellt eine wichtige Grundlage für die Modellierung von Transportphänomenen in Sedimenten dar. Dieser Parameter wird jedoch nicht routinemäßig bestimmt. Dementsprechend wird sein Wert in den numerischen Modellierungsstudien oft empirisch auf 10 gesetzt, um anisotrope Situationen in Sedimenten abzubilden. Tatsächlich ist heute die hochauflösende Charakterisierung der direktionalen hydraulischen Leitfähigkeit (DHC) in Sedimenten eine nicht leicht zu lösende Aufgabe und erfordert einen hohen messtechnischen Aufwand. Aus diesem Grund wurde eine integrierte Labormethode in Form eines modifizierten Permeameterversuchs bei konstanter Druckhöhe (MCHPT) konzipiert, um die effiziente Bestimmung und Überprüfung von konsistenten DHC-Werten in feinen bis mittleren sandigen Sedimenten durchführen zu können.

Die Berücksichtigung der Anisotropie eines Grundwasserleiters ist unter anderem bedeutend bei der Untersuchung und Bewertung von Salzwasserintrusionen. Salzwasserintrusion ist ein im globalen Maßstab auftretendes Phänomen in Küstenregionen, welches erhebliche Konsequenzen für die Nutzung der natürlichen Ressourcen in diesen Gebieten hat. Salzwasserintrusion kann als eine besondere Kategorie Grundwasserkontamination angesehen werden, denn hochmineralisiertes Wasser ist für die Trinkwassergewinnung und Bewässerung landwirtschaftlicher Kulturen ungeeignet. Auch in einem Binnengrundwasserleiter im Bereich des Beelitzhofer Wasserwerkes im Südwesten von Berlin (Deutschland) ist eine zunehmende Versalzung in den meisten tief verfilterten Brunnen zu beobachten. Ein sehr dünner Film von salzigem Grundwasser (Zentimeter-Skala) wurde in fein- bis mittelkörnigen Sanden im Hangenden des unteroligozänen Rupeltons (Grundwassergeringleiter) festgestellt. Daher kann davon

ausgegangen werden, dass elsterglaziale Rinnenstrukturen einen Salzwasseraufstieg im Bereich von trinkwasserproduzierenden Brunnen erheblich begünstigen. In früheren Arbeiten konnte eine Korrelation zwischen der hydraulischen Anisotropie a, der Grundwasserabsenkung und dem Salzwasserauftstieg nachgewiesen werden. Im Rahmen der hier durchgeführten Untersuchungen konnte der Einfluss der Anisotrope a auf die Intensität der Salzwasserintrusion durch Wasserentnahme quantifiziert werden mit einem Wert von a = 2.3. Dies erfolgte mithilfe der Labormethode (MCHPT) und dem Vergleich mit dem empirischen Wert von a = 10. Hierfür wurde ein konzeptionelles hydrogeologisches Modell der lokalen Gegebenheiten im Umfeld eines Trinkwasserentnahmebrunnens erstellt und in ein numerisches dichteabhängiges Grundwasserströmungs- und -transportmodell implementiert.

Eine tatsächliche Existenz hydraulisch wirksamer Fenster im Rupelton konnte durch die Modellstudie jedoch nicht nachgewiesen werden. Deshalb werden zwei Hypothesen über geologische Bedingungen in einem Binnengrundwasserleiter getestet, nach denen es aufgrund einer Wasserförderung aus Brunnen zum Aufstieg hochmineralsierten Grundwassers kommen kann: 1) es existieren hydraulisch wirksame Fenster im Grundwassergeringleiter, und 2) es gibt zwar keine hydraulischen Fenster, jedoch tritt der Grundwassergeringleiter in sehr geringer Mächtigkeit auf.. Es bestünde hierbei theoretisch die Möglichkeit einer Diffusion des Salzwassers durch die Tonschicht und einer Salzakkumulation an der Basis des oberen Grundwasserstockwerkes. Diese beiden Hypothesen wurden daraufhin überprüft, wie stark der Einfluss der lateralen Entfernung zwischen den hydraulisch wirksamen Fenstern im Ton und dem Entnahmebrunnen ist und ob eine Diffusion von Salzwasser durch den Ton möglich ist. Hierfür wurden unterschiedliche Mächtigkeiten (0,01 m bis 100 m) des Tones betrachtet. Hypothese 1 wurde durch vier Szenarien bestätigt. Hydraulische Fenster im Rupelton können an dieser Lokation unter bestimmten Bedingungen Salzwasserintrusionen verursachen. Dagegen kann die zweite Hypothese verworfen werden, da eine mögliche Salzdiffusion durch den Ton bei einer Mächtigkeit über 1 m keine Kontamination im überlagernden Grundwasserleiter verursachen kann.

Auf Basis der nachgewiesenen Ursachen für einen Aufstieg des tiefen salzhaltigen Grundwassers wurden zwei Empfehlungen zur Optimierung des Pumpregimes entwickelt. Hierdurch kann eine Salzwasserintrusion in einen Binnengrundwasserleiter besser kontrolliert werden. In Bezug auf die Reduktion der Pumprate für die Bedingungen im Rahmen der Modellstudie wurde ein Wert von 1,39×10⁻² m³/s (50 m³/h) für gute Trinkwasserqualität (TDS-Konzentration < 0,6 kg/m³) und eine Förderrate von 5,56×10⁻³ m³/s (20 m³/h) für exzellente Trinkwasserqualität (TDS-Konzentration < 0,3 kg/m³) ermittelt. Darüber hinaus kann auch durch eine Filterstrecke, die im oberen Grundwasserleiter den hydraulischen Anschluss von Oberflächenwasser durch Uferfiltration ermöglicht, eine Salzwasserintrusion abgeschwächt werden.

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1 Introduction

1.1 Background and problem definition

1.1.1 Hydraulic anisotropy

The two-dimensional hydraulic anisotropy (a), defined as the ratio of horizontal to vertical hydraulic conductivity (K_h/K_v), is a standard parameter of hydrogeological characterization. It is commonly considered crucial to meaningfully understand an aquifer system at various scales (Paradis and Lefebvre 2013); it usually includes defining regional groundwater flow paths (Toth 1963; Freeze and Witherspoon 1967), delineating well capture zones (Zlotnik 1997; Riva et al. 2006; Barry et al. 2009), estimating recharge through aquitards or unconsolidated sediments (Rushton et al. 1992; Gerber and Howard 2000; Hart et al. 2006), especially predicting contaminant migration (Falta et al. 2005; Wu et al. 2005). However, the a value is often empirically set to 10 in the numerical modeling studies for solving anisotropic problems in sediments respectively (Reilly and Goodman 1987; Bower et al. 1999; Zlotnik et al. 2010; Jakovovic et al. 2011; Garabedian 2013), owing to the fact that one of the challenging tasks hydrogeologists face today is the high-resolution characterization of directional hydraulic conductivity (DHC) in sediments (Vienken and Dietrich 2011).

A variety of laboratory and field methods used in sediments has been reported to yield approximations of *K*, including grain size analyses (Seelheim 1880; Hazen 1892; Terzaghi 1925; Carman 1937; Kozeny 1953; Hütte 1956; Beyer 1964; Köhler 1965; Kaubisch and Fischer 1985; Kaubisch 1986; Vukovic and Soro 1992; Kasenow 2002; Chapuis 2004), permeameter tests (Hvorslev 1951; Freeze and Cherry 1979; Todd and Mays 2005), slug and bail tests (Cooper et al. 1967; Bouwer and Rice 1976; Hyder et al. 1994; Butler 1998), pumping tests (Theis 1935; Cooper Jr and Jacob 1946; Chow 1952; Neuman 1975; Moench 1995) and borehole flow-meter tests (Molz et al. 1994; Young and Pearson 1995; Molz and Melville 1996). However, comparison of the *K* values obtained by diverse methods is difficult due to the fact that determined *K* values represent different spatial

scales and, what is more important, they all fail to measure DHC consistently. Thus, an appropriate method for measuring DHC in sediments and therefore K_v and K_h consistently is highly desirable.

Because of the fact that measuring DHC requires undisturbed samples, permeameter tests arise as an appropriate method. They have been demonstrated to be (1) suitable for a sample size of centimeters to decimeters (Wojnar et al. 2013), (2) reliable with regard to measurement precision (Paradis and Lefebvre 2013), (3) controllable over sample saturation (Madsen et al. 2008), and (4) economical with low-cost devices (Fallico et al. 2010).

With regard to sandy samples, the constant-head permeameter test (CHPT) is widely used as a standard method in the laboratory, based on the measurement of the one-dimensional steady-state water flow through a sample with a constant hydraulic gradient and the direct application of the Darcy equation to investigate K (Klute and Dirksen 1986; Xiang 1994). Considering sandy soils, the two-core method (Dabney and Selim 1987; Bathke and Cassel 1991; Dorner and Horn 2006; Petersen et al. 2008) and the modified cube method (Beckwith et al. 2003; Bagarello et al. 2009) are commonly used in CHPT for obtaining undisturbed samples to secure the values of DHC. However, both of these are only practical for sampling near-surface soil rather than at greater depths (Bagarello et al. 2009). The preliminary investigations in fine-to-medium sandy sediments have shown that CHPT is still unsuitable for consistently determining the DHC of samples with different sizes. Moreover, a precise and standardized procedure for preparing the experimental setup has not yet been reported, e.g. for dimensioning the tubing to ensure laminar flow conditions, as required for a Darcy equation-based method. Hence, it is essential to modify CHPT to be able to measure DHC in fine-to-medium sandy sediments with variable sample sizes of centimeters to decimeters consistently (Problem 1).

1.1.2 Saltwater intrusion

Saltwater intrusion is a widespread problem of continuing great practical interest in many coastal and inland aquifers all over the world, which is often described by coupled density-dependent groundwater flow and advection–dispersion equations because of hydrodynamic dispersion and a wide transition zone (Bear 1972; Huyakorn and Pinder 1983; Segol 1994; Servan-Camas and Tsai 2009; Mastrocicco et al. 2012). It is considered a special category of contamination to make groundwater unsuitable for human, industry and irrigation uses (El Moujabber et al. 2006; Abd-Elhamid and Javadi 2011).

There is an increasingly significant effect of salinization in most abstraction wells with a great depth of ~ 50 m below the surface in an inland aquifer at the Beelitzhof waterworks (BEEWW) in southwestern Berlin (Germany) (Figure 1-1), so it could be assumed that saltwater upconing, defined as the vertical upward movement of saline groundwater below a pumping well in the shape of a cone into fresh groundwater (Reilly and Goodman 1987), would come from deeper saline groundwater. This assumption is supported by geological conditions in the Northern German Basin, where the upper fresh groundwater bearing Quaternary sediments is separated from deeper saline groundwater by Oligocene clay, whose local name in the area of Berlin is Tertiary Rupelian clay (Figure 1-2). Deep reaching Quaternary Elsterian glacial erosional channels lead to either more or less thinning of the Oligocene clay up to a complete removal. Noting that a very thin film of saline groundwater (centimeter scale) has been observed in unconsolidated fluvial fine-to-medium sandy sediments on the top of the Rupelian clay at the site, therefore, it could be assumed that Elsterian glacial channels would be in the close vicinity of the site, which results in saltwater upconing owing to pressure release by pumping a large amount of groundwater in drinking-water-production wells.

As known, detailed information on a can provide an important fundament for modeling transport phenomena in sediments (Petersen et al. 2008). Thus, it is important to reveal the impact of a on saltwater intrusion in an inland aquifer due to pumping based on its precise quantification in comparison with the empirical value of 10 (Problem 2).

Chapter 1:

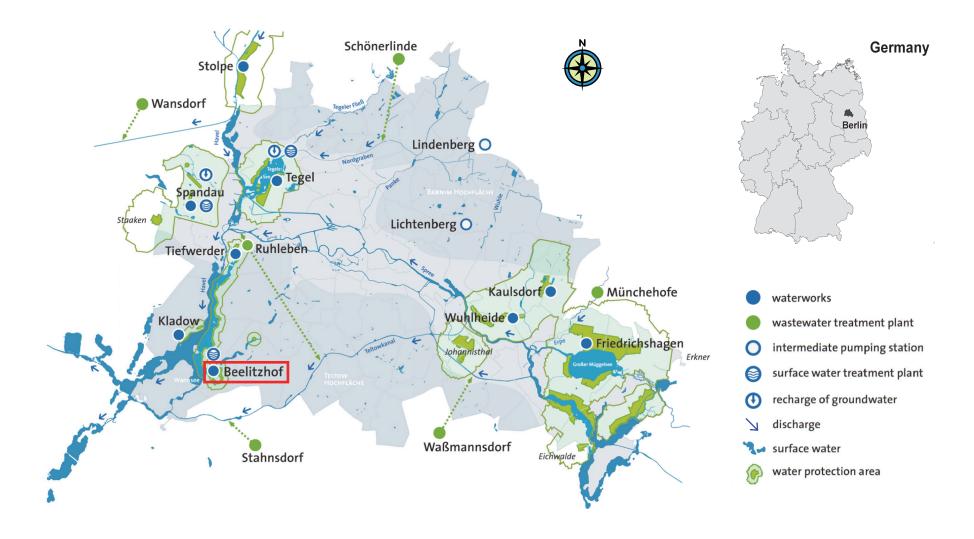


Figure 1-1 Location of field site (not to scale) (modified from Berliner Wasserbetriebe 2013).

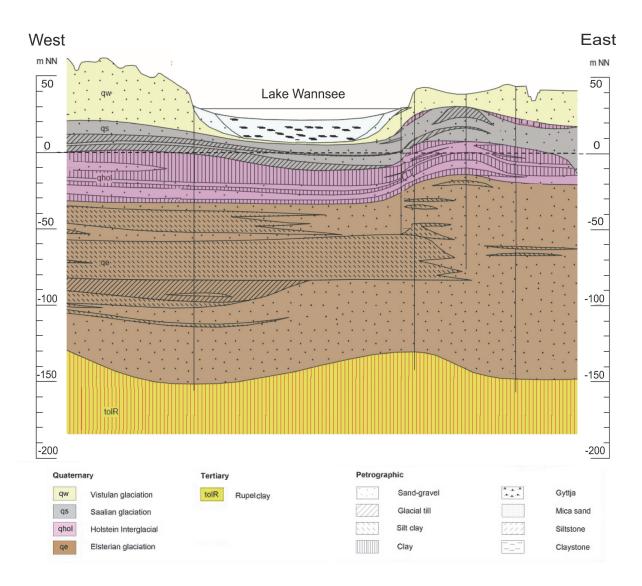


Figure 1-2 Geological profile at the site (not to scale).

As noted in many aquifers, fresh groundwater overlies denser saline groundwater (Motz 1992). However, the sources of saltwater intrusion in inland aquifers are not routinely certain in comparison with coastal aquifers that are in hydraulic connection with the sea (Freeze and Cherry 1979; Sherif et al. 1990). Saltwater intrusion in inland aquifers may originate from various sources, including (1) seawater that entered aquifers during deposition or during a high stand of the sea in past geologic time (connate water), (2) salt in saline domes, thin beds, or disseminated in the geologic formations, (3) slightly saline water concentrated by evaporation in tidal lagoon, playas, or other enclosed areas, (4) return flows to streams from irrigated lands, and (5) anthropogenic saline wastes (Bobba

1993). Accordingly, it has been found during the aforementioned modeling study that it is not yet able to be proven at the site whether there are hydraulic windows in the clay caused by glacial erosion or not. Therefore, two hypotheses about geological conditions in an inland aquifer leading to pathways for upwelling deep saline groundwater due to pumping, have arisen as to: (1) there are windows in the clay, where their locations are uncertain; and (2) there are no windows in the clay, but the clay is partially thinned out but not completely removed by glacial erosion, so salt can merely come through the clay upwards by diffusion and eventually accumulate on its top. Consequently, <u>it is interesting and necessary to reveal the impact of deep saline-groundwater sources on saltwater intrusion in an inland aquifer due to pumping (Problem 3).</u>

Saltwater intrusion can reduce freshwater storage and in extreme cases even result in abandonment of drinking-water-supply wells, if salinity, generally defined as concentration of total dissolved solids (TDS), exceeds acceptable drinking water standard (El Moujabber et al. 2006; Abd-Elhamid and Javadi 2011). Therefore, it is crucial to properly manage groundwater resources for drinking-water supply by controlling saltwater intrusion.

An enormous amount of studies in coastal aquifers has been conducted to control saltwater intrusion using various methods, which can be summarized as (1) reduction of pumping rates or rearrangement of pumping pattern, (2) relocation of pumping wells, (3) use of natural or artificial recharge, (4) construction of artificial subsurface barriers, (5) abstraction of saline water, and (6) combination of various techniques (Todd and Mays 2005; Abarca et al. 2006; Abd-Elhamid and Javadi 2011). Despite the fact that these aforementioned methods all have some constraints, the first alternative of pumping optimization has been proven more effective and economic using analytical or numerical models (Finney et al. 1992; Hallaji and Yazicigil 1996; Emch and Yeh 1998; Das and Datta 1999a, 1999b; Cheng et al. 2000; Gordon et al. 2000; Mantoglou 2003; Zhou et al. 2003; Abarca et al. 2006). In brief, the key issue of pumping optimization is to maintain a balance between pumping demand and quality requirements, it is thus essential to develop appropriate models as above mentioned for determination of water quantity which can be

pumped from aquifers while protecting pumping wells from saltwater intrusion (Mantoglou 2003; Abarca et al. 2006).

However, to date, there is greatly limited discussion for controlling saltwater intrusion in inland aquifers. Hence, <u>it is highly desirable to provide recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply based on the validated source(s) of saltwater intrusion and pumping optimization (Problem 4).</u>

1.2 Objectives of this thesis

The principal aim of this thesis is to conduct an integrated study of hydraulic anisotropy and its impact on saltwater intrusion in an inland aquifer, which includes (1) establishing a new laboratory method for the efficient determination and verification of consistent DHC values in fine-to-medium sandy sediments, (2) modeling the impact of *a* as well as deep saline-groundwater sources on saltwater intrusion due to pumping, and (3) providing recommendations of controlling saltwater intrusion for drinking-water supply.

The specific objectives of each research problem are respectively present as follows:

Problem 1

- To develop a new method to obtain undisturbed core samples with several centimeters to decimeters in length;
- To modify the experimental setup and procedure of CHPT to determine consistent K_h and K_v values with different sample sizes;
- To validate the accuracy of the developed method and modifications; and
- To provide an efficient, precise, and applicable methodological framework for general determination and verification of DHC values in fine-to-medium sandy sediments.

Problem 2

Chapter 1:

- To develop a conceptual model representative of the field situation and implement it in a numerical density-dependent groundwater flow and solute transport model;
- To assess the impacts of longitudinal and transverse dispersivity on saltwater intrusion for estimation of their uncertain values; and
- To validate the impact of a on saltwater intrusion on the basis of its precise quantification in comparison with the empirical value of 10.

Problem 3

- To validate the impact of the lateral distance between windows in the clay and the well on saltwater intrusion by testing for hypothesis 1; and
- To validate the impact of salt diffusion through the clay depending on its thickness on saltwater intrusion by testing for hypothesis 2.

Problem 4

- To reduce the pumping rate until getting the optimal value for eliminating the effect of saltwater intrusion; and
- To rearrange the pumping pattern by modifying the well construction for eliminating the effect of saltwater intrusion.

1.3 Outline of this thesis

This thesis is composed of six chapters.

Chapter 1 is the introduction of this thesis, which describes the background and problem definition as well as addresses its objectives.

The following four core chapters (Chapters 2 to 5) comprise the main research work conducted within this thesis. They have been written as manuscripts for publication in international peer-reviewed scientific journals and accordingly, each of them can be independently read as self-contained pieces of work. Therefore, they have fulfilled the

formal requirements of a cumulative dissertation. Since certain repetitions such as sections discussing background, study site, methods and results are inherent in the nature of a cumulative dissertation, a certain amount of recurrence in this thesis is inevitable. For a consistent layout, these four manuscripts have been re-edited as follows:

• Chapter 2: Laboratory method

is published as:

Jialiang Cai, Thomas Taute, Enrico Hamann, Michael Schneider (2014). *An integrated laboratory method to measure and verify directional hydraulic conductivity in fine-to-medium sandy sediments*. Ground Water. http://dx.doi.org/10.1111/gwat.12156.

This chapter proposes to establish an integrated laboratory method, called modified CHPT (MCHPT), for the efficient determination and verification of consistent DHC values in fine-to-medium sandy sediments based on a new methodological framework.

As the first author to this paper, I have been in charge of the development and conduction of the research work described as well as responsible for the scientific content and the preparation of manuscript, including literature review, data interpretation, preparation of figures and tables, and manuscript writing. Co-authors have mainly played an advisory and supervisory role.

• Chapter 3: Modeling study I

Impact of hydraulic anisotropy on saltwater intrusion

is under review as:

Jialiang Cai, Thomas Taute, Michael Schneider. *A theoretical modeling study on impact of hydraulic anisotropy on saltwater intrusion*. Environmental and Engineering Geoscience.

This chapter proposes to demonstrate the impact of a on the intensity of saltwater intrusion in an inland aquifer due to pumping based on its precise quantification in comparison with the empirical value of 10, by developing a conceptual model representative of the field

situation and implementing it in a numerical density-dependent groundwater flow and solute transport model.

As the first author to this paper, I have been in charge of the development and conduction of the research work described as well as responsible for the scientific content and the preparation of manuscript, including literature review, data interpretation, preparation of figures and tables, and manuscript writing. Co-authors have mainly played an advisory and supervisory role.

• Chapter 4: Modeling study II

Impact of deep saline-groundwater sources on saltwater intrusion is published as:

Jialiang Cai, Thomas Taute, Michael Schneider. *Saltwater upconing below a pumping well in an inland aquifer: A theoretical modeling study on testing different scenarios of deep saline-groundwater pathways*. Water, Air, & Soil Pollution. http://dx.doi.org/10.1007/s11270-014-2203-7.

This chapter proposes to test for two hypotheses about pathways of deep saline groundwater leading to saltwater upconing below a pumping well in an inland aquifer, using a density-dependent groundwater flow and solute transport model.

As the first author to this paper, I have been in charge of the development and conduction of the research work described as well as responsible for the scientific content and the preparation of manuscript, including literature review, data interpretation, preparation of figures and tables, and manuscript writing. Co-authors have mainly played an advisory and supervisory role.

• Chapter 5: Recommendations

is under review as:

Jialiang Cai, Thomas Taute, Michael Schneider. Recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply at a certain waterworks site. Environmental Earth Sciences.

This chapter proposes to provide recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply based on the validated source of saltwater intrusion and pumping optimization, using a density-dependent groundwater flow and solute transport model.

As the first author to this paper, I have been in charge of the development and conduction of the research work described as well as responsible for the scientific content and the preparation of manuscript, including literature review, data interpretation, preparation of figures and tables, and manuscript writing. Co-authors have mainly played an advisory and supervisory role.

Chapter 6 presents the conclusions of this thesis, by summarizing the major outcomes of the aforementioned core chapters and the highlights of this thesis, as well as providing an outlook for the future research.

Appendix contains additional figures that have been included in the original manuscript (Chapters 3) as supplementary material.

2 Laboratory method

The constant-head permeameter test (CHPT) is widely used in sandy samples as a standard method in the laboratory to investigate hydraulic conductivity (K). However, it neither can be used to consistently determine directional hydraulic conductivity (DHC) nor guarantee the comparability of measured K values of samples with different sizes. Therefore, this paper proposes an integrated laboratory method, called modified CHPT (MCHPT), for the efficient determination and verification of consistent DHC values in fine-to-medium sandy sediments, based on a new methodological framework. A precise and standardized procedure for preparing the experimental setup of MCHPT was conducted, based on the integrated experimental setup of CHPT and tracer tests. Moreover, a formula was yielded for the time-optimized sample saturation control. In comparison with grain-size based methods, the validity of consistent K_h and K_ν values determined by MCHPT was convincing.

Jialiang Cai, Thomas Taute, Enrico Hamann, Michael Schneider (2014)

An integrated laboratory method to measure and verify directional hydraulic conductivity in fine-to-medium sandy sediments.

Ground Water, http://dx.doi.org/10.1111/gwat.12156.

Due to copyright, the detailed information of Chapter 2 (pages 17 to 38) is not published in the online version.

Please check it via http://dx.doi.org/10.1111/gwat.12156.

3 Modeling study I: Impact of hydraulic anisotropy on saltwater intrusion

Hydraulic anisotropy (a) as a standard parameter of hydrogeological characterization can provide an important fundament for modeling transport phenomena in sediments. However, it is not routinely determined. An integrated laboratory method called modified constant-head permeameter test (MCHPT) has been developed to yield an a value of 2.3 for samples with fine-to-medium sandy sediments from an inland freshwater aguifer at the Beelitzhof waterworks in southwestern Berlin, Germany. At the site there is an increasingly significant effect of salinization in most abstraction wells with a great depth, however, the a value is often empirically set to 10 in the numerical modeling studies for solving anisotropic problems of saltwater intrusion in pumping wells. Therefore, this paper conducted a theoretical modeling study to demonstrate the impact of a on the intensity of saltwater intrusion in a pumping well based on its precise quantification. A conceptual model representative of the field situation was developed and implemented in a numerical density-dependent groundwater flow and solute transport model. Due to the hydrogeological conditions at the site, it was validated that the impact of a on saltwater intrusion was not significant. Nevertheless, the a value yielded by MCHPT provided more accurate simulations for solving anisotropic problems of saltwater intrusion in pumping wells.

Jialiang Cai, Thomas Taute, Michael Schneider

A theoretical modeling study on impact of hydraulic anisotropy on saltwater intrusion.

Submitted to Environmental and Engineering Geoscience (under review).

3.1 Introduction

The two-dimensional hydraulic anisotropy (a), defined as the ratio of horizontal to vertical hydraulic conductivity (K_h/K_v), is a standard parameter of hydrogeological characterization. It is commonly considered crucial to meaningfully understand an aquifer system at various scales (Paradis and Lefebvre 2013); it usually includes defining regional groundwater flow paths (Toth 1963; Freeze and Witherspoon 1967), delineating well capture zones (Zlotnik 1997; Riva et al. 2006; Barry et al. 2009), estimating recharge through aquitards or unconsolidated sediments (Rushton et al. 1992; Gerber and Howard 2000; Hart et al. 2006), especially predicting contaminant migration (Falta et al. 2005; Wu et al. 2005). Therefore, detailed information on a can provide an important fundament for modeling transport phenomena in sediments (Petersen et al. 2008).

Various laboratory and field methods have been used to measure a in streambeds (Chen 2000), as well as in peaty soils (Chason and Siegel 1986; Schlotzhauer and Price 1999; Beckwith et al. 2003; Surridge et al. 2005), mineral soils (Bouma and Dekker 1981; Dabney and Selim 1987; Bathke and Cassel 1991; Caris and Van Asch 1991), and sandy-loam soils (Petersen et al. 2008; Bagarello et al. 2009; Soracco et al. 2010). Concerning sandy soils, its measurements are strongly affected by heterogeneity of soil composition as well as soil structure, which leads to somewhat contradictory results (Petersen et al. 2008). Some authors pointed out that K_{ν} values were greater than K_h values, particularly in well-structured soils (Bouma 1982; Hartge 984; Bathke and Cassel 1991); while other authors reported that K_h values were greater than K_{ν} values, primarily in layered soils (Kanwar et al. 1989; Zhang 1996) or compacted soils (Dörner and Horn 2006). Hence, a is not routinely determined, because practical and validated methods are still lacking (Bagarello et al. 2009). Furthermore, specific measurements with regard to the effects of the experimental setup and procedure on determination of a in sandy sediments are rare and it is thus evidently essential to develop an appropriate method for measuring a in sandy sediments.

Chapter 3:

Cai et al. (2014a) have developed an integrated laboratory method, called modified constant-head permeameter test (MCHPT), to yield an *a* value of 2.3 for samples with Pleistocene unconsolidated fluvial fine-to-medium sandy sediments from an inland freshwater aquifer. However, the a value is often empirically set to 10 in the numerical modeling studies for solving anisotropic problems of saltwater intrusion in pumping wells (Reilly and Goodman 1987; Bower et al. 1999; Zlotnik et al. 2010; Jakovovic et al. 2011; Garabedian 2013). It is, consequently, important to reveal the impact of *a* on saltwater intrusion due to pumping based on its precise quantification in comparison with the empirical value of 10.

The principal aim of this research, thus, was to a theoretical modeling study to demonstrate the impact of *a* on the intensity of saltwater intrusion in an inland aquifer due to pumping. For that purpose, a conceptual model was developed and implemented in a numerical density-dependent groundwater flow and solute transport model.

3.2 Methods

3.2.1 Field site

There is an increasingly significant effect of salinization in most abstraction wells with a great depth of ~ 50 m below the surface in an inland aquifer at the Beelitzhof waterworks (BEEWW) in southwestern Berlin (Germany) (Figure 1-1), so it could be assumed that saltwater upconing, defined as the vertical upward movement of saline groundwater below a pumping well in the shape of a cone into fresh groundwater (Reilly and Goodman 1987), would come from deeper saline groundwater. This assumption is supported by geological conditions in the Northern German Basin, where the upper fresh groundwater bearing Quaternary sediments is separated from deeper saline groundwater by Oligocene clay, whose local name in the area of Berlin is Tertiary Rupelian clay (Figure 1-2). Deep reaching Quaternary Elsterian glacial erosional channels lead to either more or less thinning of the Oligocene clay up to a complete removal. Noting that a very thin film of

saline groundwater (centimeter scale) has been observed in unconsolidated fluvial fine-to-medium sandy sediments on the top of the Rupelian clay at the site, therefore, it could be assumed that Elsterian glacial channels would be in the close vicinity of the site, which results in saltwater upconing owing to pressure release by pumping a large amount of groundwater in drinking-water-production wells.

3.2.2 Conceptual model

According to stratigraphic investigations at the site, the geological profile (Figure 1-2) shows that an aquitard (Holstein) divides the entire fresh groundwater aquifer into an upper aquifer and a lower aquifer. Therefore, it was assumed that a well with a depth of 50 m below the surface screened in the lower aquifer would be hydraulically decoupled from the upper aquifer and Lake Wannsee (Figure 3-1). In other words, no bank filtration from the lake to the well would occur. A conceptual model (Figure 3-1) was, consequently, developed to correspond with the lower aquifer at the site as a confined unit.

Despite the observed thin film of saline groundwater in sediments on the top of the clay, it is not clear whether there are hydraulic windows in the clay caused by glacial erosion, which leads to saltwater rising and layering below freshwater in the aquifer, or only saltwater diffusion through the clay occurs, which is partially thinned out but not completely removed by glacial erosion. For simplification, thus, it was assumed that the bottom of the aquifer would be completely filled with saline groundwater and an unlimited delivery over the bottom boundary would be possible. In the case of diffusion, this assumption would lead to an overestimation of saltwater upconing.

Considering recharge rate (*E*) (Figure 3-1), its areal effects on the critical rise were small enough ($E/K_v = 7.29 \times 10^{-5}$) to be excluded from the analysis (Garabedian 2013).

3.2.3 Numerical model development

Chapter 3:

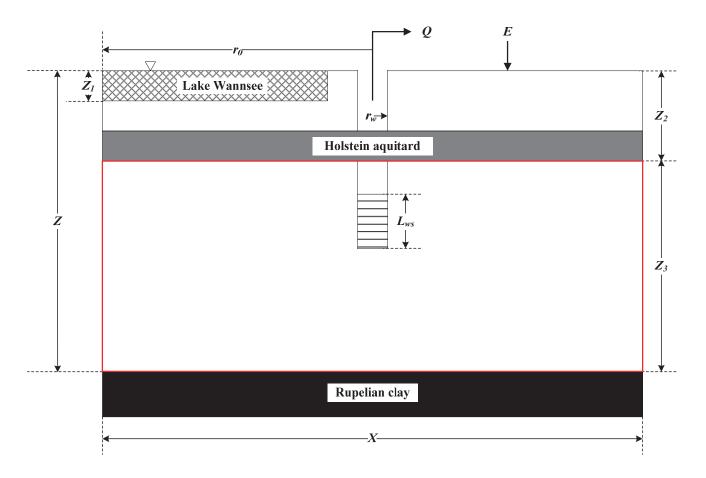


Figure 3-1 Schematic vertical cross-section of field situation and conceptual model (red rectangular area) (not to scale). X - model width, 2000 m; Z_3 - thickness of the lower fresh groundwater aquifer (model height), 140 m; Z - thickness of the entire fresh groundwater aquifer, 170 m; Z_1 - depth of Lake Wannsee, 9 m; Z_2 - thickness of the upper fresh groundwater aquifer, 30 m; r_w - well radius, 0.45 m; L_{ws} - length of well screen, 30 m; r_0 - radial distance from well center to constant head boundary condition, 1000 m; Q - pumping rate, 2.78×10^{-2} m^3/s ; E - recharge rate, 3.17×10^{-9} m/s.

Numerical modeling was performed using SEAWAT-2000 (Langevin et al. 2007). SEAWAT-2000 is a coupling of the MODFLOW groundwater flow code, modified to solve variable-density flow conditions using equivalent freshwater head, with the MT3DMS transport model (Garabedian, 2013). The coupling between fluid density and solute concentration is incorporated in the code as a linear relationship.

3.2.2.1 Model discretization

Despite the fact that three-dimensional conditions were obtained in the conceptual model, the model was simplified into a two-dimensional X-Z environment to diminish the computational effort (Jakovovic et al. 2011). The model was spatially discretized to form a nonuniform mesh. The columns (Δx) were variably spaced with 0.45-m horizontal resolution at the well according to the well radius (r_w) of 0.45 m at the site symmetrically expanding to 20-m horizontal resolution at the lateral boundaries (Figure 3-1). The layers (Δz) were spaced into two parts: (1) each layer was set to 10 m thick above the well screen (5 layers total); (2) each layer was set to 2 m thick below the well screen (45 layers total) (Figure 3-1). In order to minimize numerical dispersion and oscillation, the common criterion mesh Peclet number (Pe) was set to be ≤ 2 with all different Δx values (Zheng and Bennett 2002).

All simulations were performed as transient flow until steady-state conditions were reached, using the TVD advection solver, which is mass conservative, without excessive numerical dispersion and artificial oscillation (Zheng and Bennett 2002). Trial-and-error analysis demonstrated that it took 600 years to reach steady-state conditions with the current model setup, where time steps (Δt) were set to 1 year. Using this small Δt value can ensure that Courant number (Cr) correspondingly remained \leq 1 with all different Δx values for minimization of numerical dispersion and oscillation (Zheng and Bennett 2002).

3.2.2.2 Boundary and initial conditions

The top of the model was set to no-flow boundaries according to the Holstein aquitard (Figure 3-1). The left- and right-hand sides of the model were chosen to be far enough (r_w/r_0) (the radial distance from the well center to the constant head boundary condition) = 4.5×10^{-4}) (Figure 3-1) not to be influenced by the pumping activities (Jakovovic et al. 2011; Garabedian 2013) and implemented as 1^{st} order boundary conditions with a constant head $(h_0 = 30 \text{ m})$ and concentration $(C_0 = 0.2 \text{ kg/m}^3)$ respectively. According to the observed thin film of saline groundwater in sediments on the top of the impermeable Rupelian clay, 2^{nd} order boundary conditions were chosen at the bottom of the model.

The simulated concentration was obtained at the bottom of the well screen. The concentration of saline groundwater (C_I) was incorporated as total dissolved solid (TDS). Its value was set to 5.5 kg/m³ according to the aforementioned observed thin film of saline groundwater at the site.

3.2.2.3 Model parameters

The model was considered to be homogeneous according to Cai et al. (2014a), with uniform parameters. The site-specified values of h_0 , hydraulic gradient (i), K_h , specific storage (S_s) and effective porosity (n_e) were measured (Table 3-1). Due to the fact that longitudinal and transverse dispersivity were uncertain, it was therefore essential to assess their impacts on saltwater intrusion. Longitudinal dispersivity (α_L) is an intrinsic property of the aquifer and it is found in practice to be dependent on and proportional to the scale of the measurement (Konikow 2011). Most reported values of α_L are in a range from 0.01 to 1.0 times the scale of the measurement, albeit the ratio of α_L to scale of measurement tends to decrease at larger scales (Anderson 1984; Gelhar et al. 1992; Frippiat and Holeyman 2008). With regard to transverse dispersivity (α_T), it is commonly assumed to be approximately one to three orders of magnitude smaller than α_L (Harleman and Rumer 1963; Zheng and Bennett 2002; Huang et al. 2003; Jakovovic et al 2011). Consequently, an assessment of the impacts of α_L and α_T was conducted with values varying in a range from 0.5 to 20 m and from 0.01 to 1 m respectively.

Table 3-1 Numerical model parameters

Para	meter	Symbol	Value	Unit
	Model width	X	2000	m
	Model height	Z_3	140	m
	Initial hydraulic head	h_0	30	m
eter	Hydraulic gradient	i	0	-
Flow Parameter	Horizontal hydraulic conductivity	K_h	1×10 ⁻⁴	m/s
w Ра	Hydraulic anisotropy	a	1, 2.3, 10	-
Flo	Effective porosity	n_e	0.3	-
	Well radius	r_w	0.45	m
	Length of well screen	L_{ws}	30	m
	Pumping rate	Q	2.78×10 ⁻²	m^3/s
	Specific storage	S_s	5×10 ⁻⁴	1/m
eter	Longitudinal dispersivity	a_L	0.5, 1, 5, 10, 20	m
ıram	Transverse dispersivity	α_T	0.01, 0.05, 0.1, 0.5, 1	m
rt Pa	Effective diffusion coefficient in porous media	D^*	1×10 ⁻¹⁰	m^2/s
Transport Parameter	Total dissolved solids (TDS) concentration of		0.2	1r or /
Tra	fresh groundwater	C_{θ}	0.2	kg/m
	TDS concentration of saline groundwater	C_I	5.5	kg/m

Table 3-2 Water classification by total dissolved solids (TDS) concentration (Masters and Ela 2008)

Classification	TDS Concentration (kg/m³)
Freshwater	<1
Brackish water	1~10
Saline water	10~30
Brine	>30

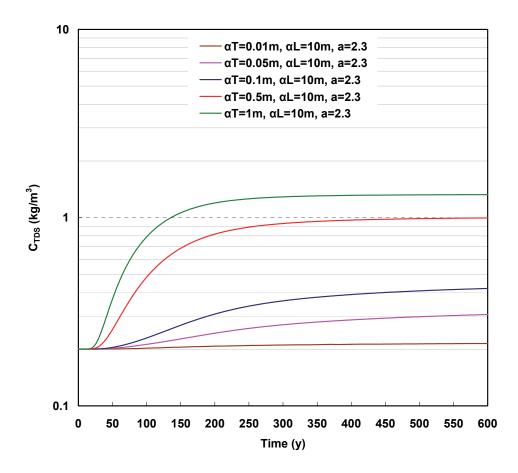


Figure 3-2 Total dissolved solids (TDS) concentration at the bottom of the well screen with varying transverse dispersivity (α_T). (1) Longitudinal dispersivity (α_L) and hydraulic anisotropy (a) were set to constant values of 10 m and 2.3 respectively; (2) the dashed line represents the concentration threshold between freshwater and brackish water.

3.3 Results and discussion

3.3.1 Impact of dispersivity

There were 5 scenarios simulated by variable α_T values (Figure 3-2). When $\alpha_T = 1$ m, the salinity in the well was > 1 kg/m³; when $\alpha_T = 0.5$ m, the salinity was nearly equal to 1 kg/m³; when $\alpha_T = 0.01$, 0.05 and 0.1 m, the salinity was all < 1 kg/m³. Accordingly, all simulations at 20%, 50% and 80% concentration contour of C_I enormously differed from each other as well (Figure A-1). The concentration distribution for saltwater upconing is therefore very sensitive to α_T (Reilly and Goodman 1987). Noting the criteria listed in Table 3-2, the well water with α_T values of 0.01, 0.05, 0.1 and 0.5 m was still classified as

freshwater, which indicated that there would be slight or modest effect of saltwater intrusion, whereas only with α_T value of 1 m was consistent with the situation that significant effect of saltwater intrusion occurs at the site.

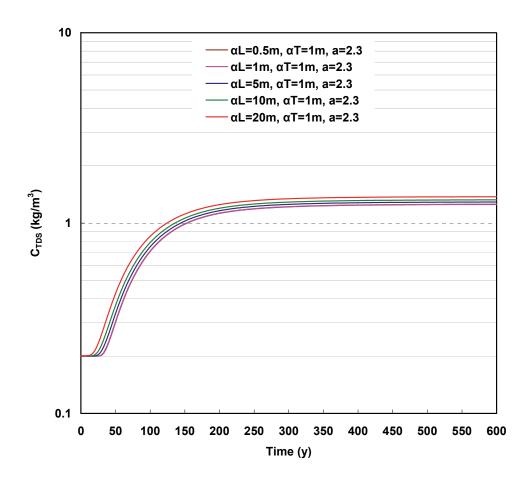


Figure 3-3 Total dissolved solids (TDS) concentration at the bottom of the well screen with varying longitudinal dispersivity (α_L). (1) Transverse dispersivity (α_T) and hydraulic anisotropy (a) were set to constant values of 1 m and 2.3 respectively; (2) the dashed line represents the concentration threshold between freshwater and brackish water.

As shown in Figure 3-3, the salinity in the well simulated by variable α_L values was all > 1 kg/m³ within a very small range. Correspondingly, all simulations at 20%, 50% and 80% concentration contour of C_I were almost identical as well (Figure A-2). Thus, α_L does not play a major role in determining the preceding concentration distribution (Reilly and Goodman 1987). Meanwhile, the well water of all simulations was classified as brackish water, with consistency in the significant effect of saltwater intrusion at the site. Due to Pe

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defined as the ratio of Δx to α_L , α_L values of 10 and 20 m could both ensure that Pe was ≤ 2 with all different Δx values. However, smaller values generally produce satisfactory simulations (Zheng and Bennett 2002; Jakovovic et al. 2011).

Consequently, the α_L and α_T values were estimated to 10 and 1 m respectively, according to their impacts on saltwater intrusion.

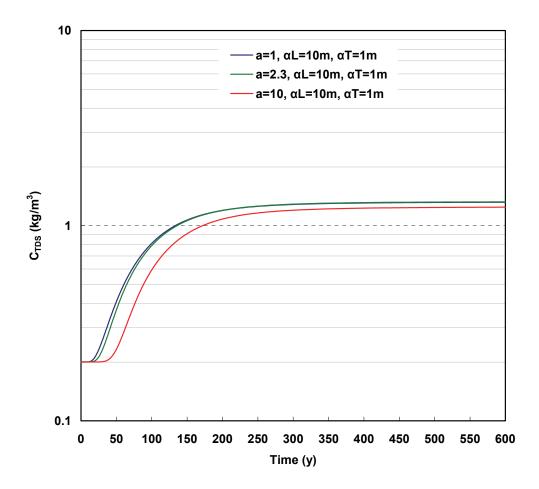


Figure 3-4 Total dissolved solids (TDS) concentration at the bottom of the well screen with varying hydraulic anisotropy (a). (1) Longitudinal dispersivity (α_L) and transverse dispersivity (α_T) were set to constant values of 10 m and 1 m respectively; (2) the dashed line represents the concentration threshold between freshwater and brackish water.

3.3.2 Impact of hydraulic anisotropy

Figure 3-4 indicated that the salinity in the well simulated by variable a values was all > 1

kg/m³, so that the well water of all simulations was classified as brackish water, which was consistent with the aforementioned observation at the site. Meanwhile, all simulations at 20%, 50% and 80% concentration contour of C_1 were quite similar with only slight differences among them (Figure A-3). Therefore, the preceding concentration distribution is to some extent insensitive to a.

It is notable that Garabedian (2013) developed a new steady-state analytical solution for the saltwater upconing problem with no-flow boundary conditions at the top and bottom in a partially completed pumping well. With the assumption that r_w is much smaller than the freshwater aquifer thickness which in turn is significantly smaller than r0, this solution was evaluated for accuracy by comparison to numerical simulations in an isotropic scenario and an anisotropic scenario (a = 10) respectively. On the condition that $r_w/r_0 > 0.1$, it demonstrated that a was a sensitive parameter impacting on drawdown and correspondingly saltwater upconing, regardless of the ratio of the vertical elevation from the bottom of the freshwater aguifer to the freshwater aguifer thickness. Moreover, Garabedian (2013) also pointed out that this solution differed from that of Zlotnik et al. (2010) with the constant-potential upper boundary conditions and the no-flow lower boundary conditions. Thus, there were two assumable reasons why the impact of a on the intensity of saltwater intrusion in a pumping well was not significant in our case. On the one hand, our modeling setup was not completely consistent with the assumption of the aforementioned solution from Garabedian (2013) owing to the fact that r_0 was not significantly greater than the freshwater aquifer thickness. On the other hand, the boundary conditions in our modeling setup differed from those in Garabedian (2013) and Zlotnik et al. (2010). Hence, it could be considered to be reasonable for the hydrogeological conditions at the Beelitzhof waterworks that the impact of a on saltwater intrusion in a pumping well was not significant.

3.4 Conclusions

This research conducted a theoretical modeling study to demonstrate the impact of a on the

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intensity of saltwater intrusion in a pumping well in an inland aquifer at the Beelitzhof waterworks in southwestern Berlin, Germany. Due to the hydrogeological conditions at the site, it was validated that the impact of a on saltwater intrusion was not significant, based on its precise value of 2.3 in comparison with the empirical value of 10. Nevertheless, the a value yielded by MCHPT provided more accurate simulations for solving anisotropic problems of saltwater intrusion in pumping wells.

4 Modeling study II: Impact of deep saline-groundwater sources on saltwater intrusion

To date, studies on the geological conditions in inland aquifers leading to pathways for upwelling deep saline groundwater due to pumping have been not yet published. Therefore, this paper conducted a theoretical modeling study to raise two hypotheses about deep saline-groundwater pathways leading to saltwater upconing below a pumping well in an inland aquifer based on the field situation at the Beelitzhof waterworks in southwestern Berlin (Germany), defined as (1) there are windows in the Rupelian clay caused by glacial erosion, where their locations are uncertain; and (2) there are no windows in the clay, but the clay is partially thinned out but not completely removed by glacial erosion, so salt can merely come through the clay upwards by diffusion and eventually accumulate on its top. These hypotheses were tested to demonstrate the impact of the lateral distance between windows in the clay and the well, as well as salt diffusion through the clay depending on its thickness on saltwater intrusion in the pumping well respectively, using a density-dependent groundwater flow and solute transport model. Hypothesis 1 was validated with 4 scenarios that windows could occur in the clay at the site and their locations under some conditions could significantly cause saltwater intrusion, while hypothesis 2 could be excluded, because salt diffusion through the clay with thickness greater than 1 m at the site was not able to cause saltwater intrusion.

Jialiang Cai, Thomas Taute, Michael Schneider (2014)

Saltwater upconing below a pumping well in an inland aquifer: A theoretical modeling study on testing different scenarios of deep saline-groundwater pathways

Water, Air, & Soil Pollution, http://dx.doi.org/10.1007/s11270-014-2203-7.

4.1 Introduction

Saltwater upconing is the vertical upward movement of saline groundwater below a pumping well in the shape of a cone into fresh groundwater and is a problem of continuing great practical interest in many coastal and inland aquifers around the world (Reilly and Goodman 1987). In general, its main issue is focused on analyzing its critical condition, i.e. determining the critical pumping rate, or the pumping rate at which the cone will become unstable, as well as determining the accompanying critical rise, or the height to which the cone will rise below the pumping well before incipient instability occurs (Bower et al. 1999; Massmann et al. 2006). It has been reported by using a variety of analytical solutions (Schmorak and Mercado 1969; Haubold 1975; Motz 1992; Bower et al. 1999; Garabedian 2013) and numerical models (Chandler and McWhorter 1975; Wirojanagud and Charbeneau 1985; Reilly et al. 1987; Panday et al. 1993; Zhou et al. 2005; Garabedian 2013). Due to the challenges of undertaking field-based measurements of salt transport dynamics occurring below the pumping well, saltwater upconing research has been developed at laboratory scale rather than predominantly based on aforementioned theoretical analyses (Jakovovic et al. 2011). The laboratory experiments in the sand box (tank) were conducted to capture the behavior of saltwater upconing and correspondingly the numerical models were used to calibrate the input parameters, validate the laboratory observations, as well as provide further insight into the physical processes of saltwater upconing, which can not be perceived from physical experiments alone (Oswald 1998; Johannsen et al. 2002; Oswald and Kinzelbach 2004; Goswami and Clement 2007; Konz et al. 2009; Werner et al. 2009; Jakovovic et al 2011).

As noted in many aquifers, fresh groundwater overlies denser saline groundwater (Motz 1992). However, unlike in coastal aquifers that are in hydraulic connection with the sea, deep saline-groundwater pathways in inland aquifers are not routinely certain. To date, studies on the geological conditions in inland aquifers leading to pathways for upwelling deep saline groundwater due to pumping have been not yet published. Therefore, it is interesting and essential to reveal how deep saline-groundwater pathways impact on

saltwater upconing below a pumping well in an inland aquifer.

Our preliminary study (Chapter 3) has shown that is an increasingly significant effect of salinization in most abstraction wells with a great depth of ~ 50 m below the surface in an inland aquifer at the Beelitzhof waterworks (BEEWW) in southwestern Berlin (Germany) (Figure 1-1), so it could be assumed that saltwater upconing would come from deeper saline groundwater. This assumption is supported by geological conditions in the Northern German Basin, where the upper fresh groundwater bearing Quaternary sediments is separated from deeper saline groundwater by Oligocene clay, whose local name in the area of Berlin is Tertiary Rupelian clay (Figure 1-2). Deep reaching Quaternary Elsterian glacial erosional channels lead to either more or less thinning of the Oligocene clay up to a complete removal. Noting that a very thin film of saline groundwater (centimeter scale) has been observed in unconsolidated fluvial fine-to-medium sandy sediments on the top of the Rupelian clay at the site, therefore, it could be assumed that Elsterian glacial channels would be in the close vicinity of the site, which results in saltwater upconing owing to pressure release by pumping a large amount of groundwater in drinking-water-production wells. However, it is not yet able to be proven whether there are hydraulic windows in the clay caused by glacial erosion or not, our hypotheses about deep saline-groundwater pathways, thus, arose as to: (1) there are windows in the clay, where their locations are uncertain; and (2) there are no windows in the clay, but the clay is partially thinned out but not completely removed by glacial erosion, so salt can merely come through the clay upwards by diffusion and eventually accumulate on its top.

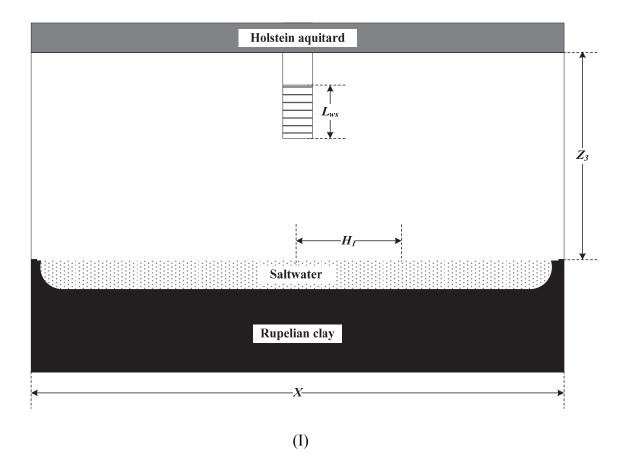
The principal aim of this research, consequently, was to conduct a theoretical study to test for two hypotheses about deep saline-groundwater pathways leading to saltwater upconing below a pumping well in an inland aquifer based on the field situation at the site, using a density-dependent groundwater flow and solute transport model. The specific objectives were to demonstrate the impact of (1) the lateral distance between windows in the clay and the well, as well as (2) salt diffusion through the clay depending on its thickness on saltwater intrusion in the pumping well.

4.2 Methods

4.2.1 Conceptual models

Our preliminary study (Chapter 3) has indicated the field situation at the site in detail, which is schematically present in Figure 3-1. Two conceptual models were thus accordingly developed in the lower aquifer as a confined unit. Each conceptual model was representative of the deep saline-groundwater pathway in the corresponding hypothesis (Figure 4-1).

The areal effects of recharge rate (E) on the critical rise were small enough to be excluded from the analysis, according to our preliminary study (Chapter 3).



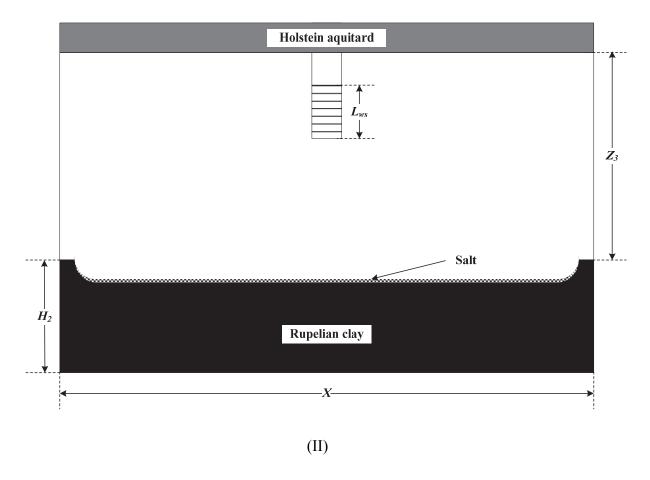
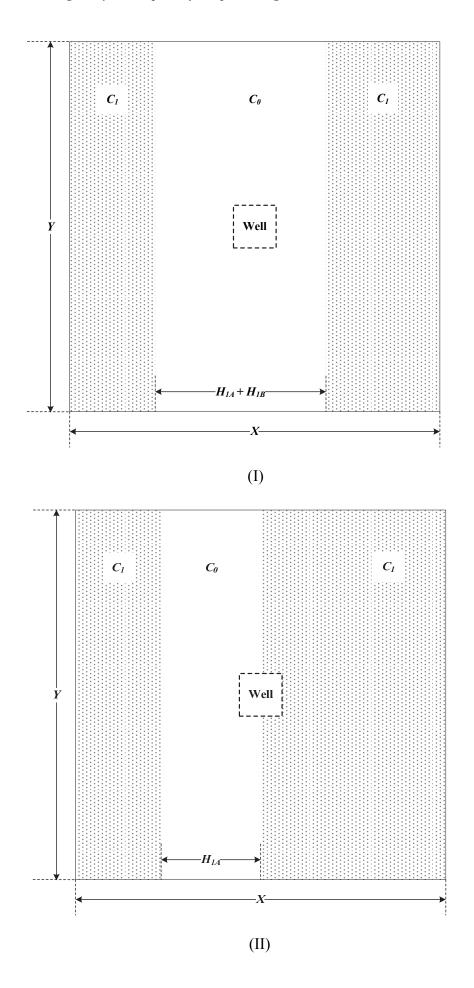


Figure 4-1 Schematic vertical cross-section of conceptual models of hypothesis 1 (I) and hypothesis 2 (II) (not to scale). X - model width; Z_3 - model height (thickness of the lower fresh groundwater aquifer); L_{ws} - length of well screen; H_1 - lateral distance from the well to windows in the Rupelian clay; H_2 - thickness of the Rupelian clay.

4.2.1.1 Conceptual model 1: Flow through erosional windows in the Rupelian clay

Four scenarios were developed to interpret hypothesis 1. They were the windows A and B were located on the left- and right-hand sides of the well respectively on condition that $H_{IA} = H_{IB}$ (Scenario 1) or $H_{IA} \neq H_{IB}$ (Scenario 2) (Figure 4-2I); the window A was only located on one side of the well on condition that $H_{IB} = 0$ (Scenario 3) (Figure 4-2II); and the window A was only located on one side of the well on condition that $H_{IB} \rightarrow +\infty$ (Scenario 4) (Figure 4-2III)



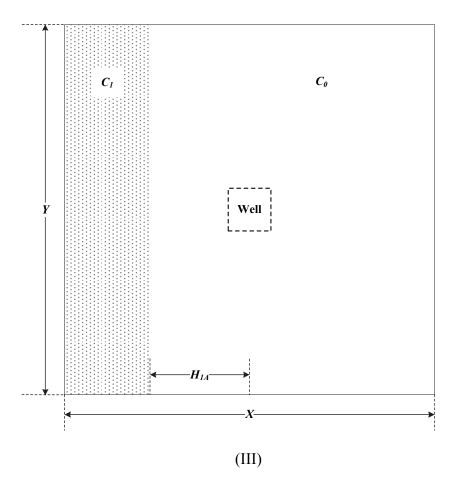


Figure 4-2 Schematic horizontal cross-section of four scenarios for interpretation of hypothesis 1 in the X-Y plane (not to scale). (I) The windows A and B were located on the left- and right-hand sides of the well respectively on condition that $H_{1A} = H_{1B}$ (Scenario 1) or $H_{1A} \neq H_{1B}$ (Scenario 2); (II) the window A was only located on one side of the well on condition that $H_{1B} = 0$ (Scenario 3); (III) the window A was only located on one side of the well on condition that $H_{1B} \to +\infty$ (Scenario 4). C_0 and C_1 represent the total dissolved solids (TDS) concentration of fresh groundwater and saline groundwater respectively.

4.2.1.2 Conceptual model 2: Diffusion through the Rupelian clay

Salt diffusion through the clay is the process in porous media whereby ionic or molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradient (Freeze and Cherry 1979). According to Fick's first law, the mass flux (*F*) was therefore used to interpret hypothesis 2. It can be two-dimensionally

expressed as

$$F = -D^* \times \Delta x \times \frac{C_0 - C_2}{H_2} \tag{4-1}$$

where D^* is the effective diffusion coefficient in porous media; Δx is the model cell width; C_0 is the total dissolved solids (TDS) concentration of fresh groundwater; C_2 is the TDS concentration of saline groundwater; H_2 is the thickness of the clay.

4.2.2 Numerical model development

Numerical modeling was performed using SEAWAT-2000 (Langevin et al. 2007). SEAWAT-2000 is a coupling of the MODFLOW groundwater flow code, modified to solve variable-density flow conditions using equivalent freshwater head, with the MT3DMS transport model (Garabedian 2013). The coupling between fluid density and solute concentration is incorporated in the code as a linear relationship. The developed numerical model in our preliminary study (Chapter 3) was used, with specified modifications for this research.

4.2.2.1 Model discretization

The model in a two-dimensional X-Z environment was spatially discretized to form a nonuniform mesh. The columns (Δx) were variably spaced with 0.45-m horizontal resolution at the well according to the well radius (r_w) of 0.45 m at the site symmetrically expanding to 20-m horizontal resolution at the lateral boundaries (Figure 3-1). The layers (Δz) were spaced into two parts: (1) each layer was set to 10 m thick above the well screen (5 layers total); (2) each layer was set to 2 m thick below the well screen (45 layers total) (Figure 3-1). In order to minimize numerical dispersion and oscillation, the common criterion mesh Peclet number (Pe) was set to be \leq 2 with all different Δx values (Zheng and Bennett 2002).

All simulations were performed as transient flow until steady-state conditions were

reached, using the TVD advection solver, which is mass conservative, without excessive numerical dispersion and artificial oscillation (Zheng and Bennett 2002). Trial-and-error analysis demonstrated that it took 600 years to reach steady-state conditions with the current model setup, where time steps (Δt) were set to 1 year. Using this small Δt value can ensure that Courant number (Cr) correspondingly remained ≤ 1 with all different Δx values for minimization of numerical dispersion and oscillation (Zheng and Bennett 2002).

4.2.2.2 Boundary and initial conditions

The top of the model was set to no-flow boundaries according to the Holstein aquitard (Figure 3-1). The left- and right-hand sides of the model were chosen to be far enough (r_w/r_0) (the radial distance from the well center to the constant head boundary condition) = 4.5×10^{-4}) (Figure 3-1) not to be influenced by the pumping activities (Jakovovic et al. 2011; Garabedian 2013) and implemented as 1st order boundary conditions with a constant head $(h_0 = 30 \text{ m})$ and concentration $(C_0 = 0.2 \text{ kg/m}^3)$ respectively. According to the observed thin film of saline groundwater in sediments on the top of the impermeable Rupelian clay, 2^{nd} order boundary conditions were chosen at the bottom of the model.

The simulated concentration was obtained at the bottom of the well screen. The concentration of saline groundwater was incorporated as total dissolved solid (TDS). Its TDS concentration in hypothesis 1 (C_1) was set to 5.5 kg/m³ according to the aforementioned observed thin film of saline groundwater at the site as well as its TDS concentration in hypothesis 2 (C_2) was set to 29.4 kg/m³ according to Assmann and Gandert (1957) as well as Wurl (1995).

4.2.2.3 Model parameters

The model was considered to be homogeneous according to Cai et al. (2014a), with uniform parameters. The site-specified values of h_0 , hydraulic gradient (i), K_h , specific storage (S_s) and effective porosity (n_e) were measured (Table 4-1). According to our preliminary study (Chapter 3), the longitudinal (α_L) and transverse dispersivity (α_T) values

were estimated to 10 and 1 m respectively. The hydraulic anisotropy (a) defined as K_h/K_v was determined to 2.3 by an integrated laboratory method called modified constant-head permeameter test (MCHPT) (Cai et al. 2014a).

Table 4-1 Numerical model parameters

Para	meter	Symbol	Value	Unit
	Model width	X	2000	m
	Model height	Z_3	140	m
	Initial hydraulic head	h_0	30	m
ster	Hydraulic gradient	i	0	-
ram(Horizontal hydraulic conductivity	K_h	1×10 ⁻⁴	m/s
Flow Parameter	Hydraulic anisotropy	а	2.3	-
Flox	Effective porosity	n_e	0.3	-
	Well radius	r_w	0.45	m
	Length of well screen	L_{ws}	30	m
	Pumping rate	Q	2.78×10 ⁻²	m^3/s
	Specific storage	S_s	5×10 ⁻⁴	1/m
	Longitudinal dispersivity	α_L	10	m
	Transverse dispersivity	α_T	1	m
er	Effective diffusion coefficient in porous media	\overline{D}^*	1×10 ⁻¹⁰	m^2/s
ransport Parameter	Total dissolved solids (TDS) concentration of fresh groundwater	C_{θ}	0.2	kg/m ³
nsport l	TDS concentration of saline groundwater in hypothesis 1	C_I	5.5	kg/m ³
Tra	TDS concentration of saline groundwater in hypothesis 2	C_2	29.4	kg/m ³
	Lateral distance from the well to windows in the Rupelian clay	H_{l}	0~1000	m
	Thickness of the Rupelian clay	H_2	0~100	m

4.3 Results and discussion

4.3.1 Testing for hypothesis 1: Variable lateral distance between erosional windows in the Rupelian clay and the well

A series of tests in Scenario 1 showed that the salinity in the well was estimated to be 1 kg/m³ when $H_{IA} = H_{IB} = 550$ m (Figure 4-3I), i.e. the well water was classified as brackish water on condition that $0 < H_{IA} = H_{IB} \le 550$ m, noting the criteria listed in Table 3-2. Owing to the waterworks site for drinking-water supply, it was essential to consider the impact of TDS concentration on the drinking water palatability (DWP) as well. According to the criteria listed in Table 4-2, DWP was classified as unacceptable on condition that $0 < H_{IA} = H_{IB} \le 400$ m, as poor on condition that 400 m $< H_{IA} = H_{IB} \le 615$ m, as fair on condition that 615 m $< H_{IA} = H_{IB} \le 805$ m, and as good on condition that 805 m $< H_{IA} = H_{IB} \le 960$ m, respectively. Thus, when $0 < H_{IA} = H_{IB} \le 550$ m, the effect of saltwater intrusion was significant, as the well water was brackish water and DWP was unacceptable to poor; when 550 m $< H_{IA} = H_{IB} \le 615$ m, the effect was modest, as the well water was freshwater but DWP was poor; when 615 m $< H_{IA} = H_{IB} \le 960$ m, there was no or slight effect, as the well water was freshwater and DWP was fair to good.

Table 4-2 Palatability classification of drinking water by total dissolved solids (TDS) concentration (WHO 2003)

Classification	TDS Concentration (kg/m³)
Excellent	< 0.3
Good	0.3~0.6
Fair	0.6~0.9
Poor	0.9~1.2
Unacceptable	>1.2

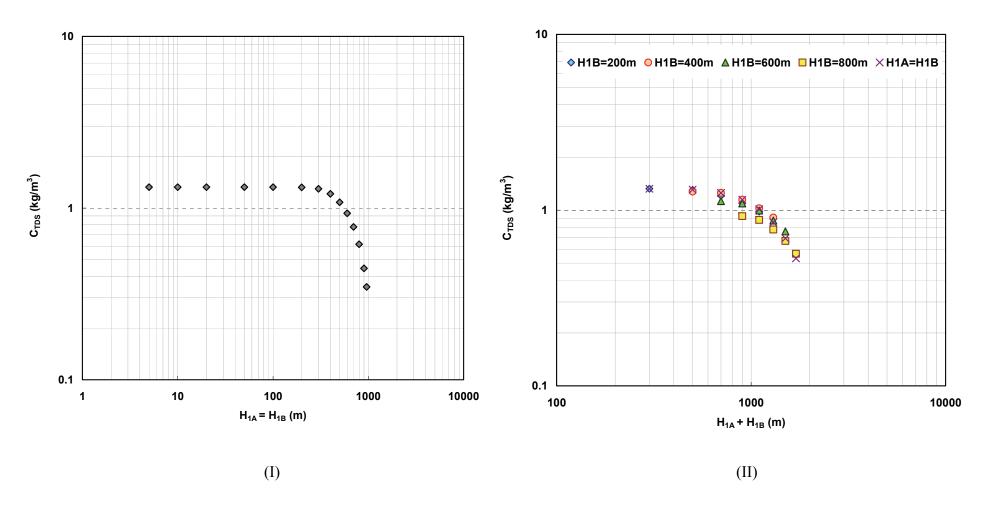


Figure 4-3 Simulations of total dissolved solids (TDS) concentration at steady-state condition in the well by Scenario 1 (I) and Scenario 2 (II) of hypothesis 1. The dashed line represents the concentration threshold between freshwater and brackish water.

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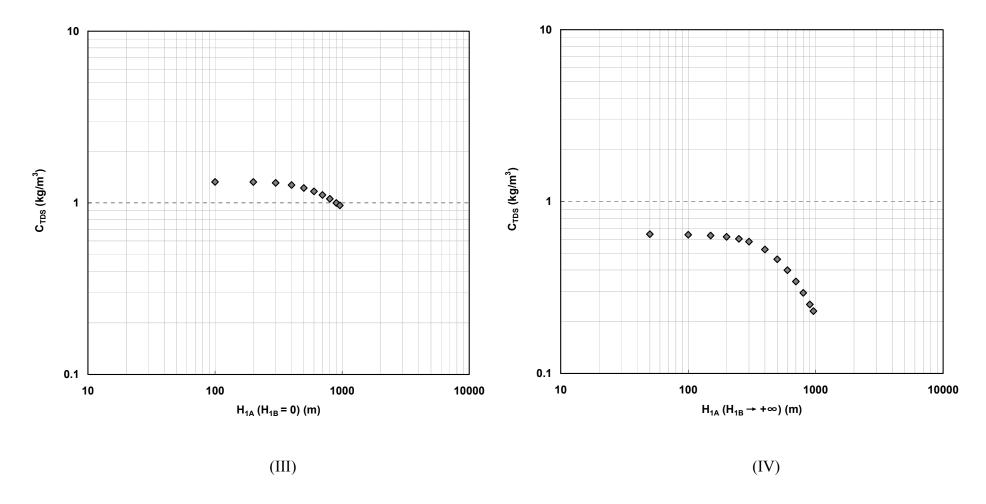


Figure 4-3 (continued) Simulations of total dissolved solids (TDS) concentration at steady-state condition in the well by Scenario 3 (III) and Scenario 4 (IV) of hypothesis 1. The dashed line represents the concentration threshold between freshwater and brackish water.

Considering Scenario 2, a series of tests yielded the greatly similar salinity in comparison to Scenario 1 (Figure 4-3II). When the $H_{IA} + H_{IB}$ values were held constant, the salinity with different combinations of H_{IA} and H_{IB} were almost exceedingly close to each other as well (Figure 4-3II). Therefore, Scenario 1 and 2 could be merged into one scenario, defined as the windows A and B were located on the left- and right-hand sides of the well respectively, without consideration of H_{IA} or H_{IB} conditions. The aforementioned results were, consequently, summarized as follows: when $0 < H_{IA} + H_{IB} \le 1100$ m, the effect of saltwater intrusion was significant, as the well water was brackish water and DWP was unacceptable to poor; when 1100 m $< H_{IA} + H_{IB} \le 1230$ m, the effect was modest, as the well water was freshwater but DWP was poor; when 1230 m $< H_{IA} + H_{IB} \le 1920$ m, there was no or slight effect, as the well water was freshwater and DWP was fair to good.

With regard to Scenario 3, a series of tests indicated that the salinity in the well was estimated to be 1 kg/m³ when $H_{IA} = 865$ m (Figure 4-3III), i.e. the well water was classified as brackish water on condition that $0 < H_{IA} \le 865$ m. DWP was classified as unacceptable on condition that $0 < H_{IA} \le 530$ m, and as poor on condition that 530 m $< H_{IA} \le 960$ m, respectively. Thus, when $0 < H_{IA} \le 865$ m, the effect of saltwater intrusion was significant, as the well water was brackish water and DWP was unacceptable to poor; when 865 m $< H_{IA} \le 960$ m, the effect was modest, as the well water was freshwater but DWP was poor.

As for Scenario 4, a series of tests demonstrated that the salinity of all simulations was < 1 kg/m³ (Figure 4-3IV), i.e. the well water of all simulations was classified as freshwater. DWP was classified as fair on condition that $0 < H_{IA} \le 265$ m, as good on condition that 265 m $< H_{IA} \le 790$ m, and as excellent on condition that 790 m $< H_{IA} \le 960$ m, respectively. Therefore, there was no or slight effect of saltwater intrusion, as the well water was freshwater and DWP was fair to excellent.

In the case of hypothesis 1, i.e. flow through erosional windows in the clay, the numerical simulations of 4 developed scenarios yielded different results for presenting the impact of

the certain lateral distance between windows in the clay and the well on saltwater intrusion. In terms of Scenario 1 and 2, there was a great consistency between these two scenarios, in which the lateral distance $H_{IA} + H_{IB}$ in the range of (0, 1230] m had a modest-to-significant impact on saltwater intrusion in the pumping well, without consideration of H_{IA} or H_{IB} conditions. In terms of Scenario 3 and 4 with two extreme conditions of H_{IB} , their results indicated a complete contrast to each other, in which the entire lateral distance H_{IA} on condition that $H_{IB} = 0$ (Scenario 3) had a modest-to-significant impact on saltwater intrusion, while the entire lateral distance H_{IA} on condition that $H_{IB} \rightarrow +\infty$ (Scenario 4) had no or a slight impact on saltwater intrusion. Consequently, it was validated that the effect of saltwater intrusion depended on the lateral distance between windows in the clay and the well, which led to the conclusion that windows could occur in the clay at the site and their locations under some conditions could significantly cause saltwater intrusion in the pumping well.

4.3.2 Testing for hypothesis 2: Salt diffusion through the Rupelian clay with variable thickness

A series of tests showed that the salinity in the well was estimated to be 1 kg/m³ when H_2 = 0.7 m (Figure 4-4), i.e. the well water was classified as brackish water on condition that 0 < $H_2 \le 0.7$ m. DWP was classified as unacceptable on condition that $0 < H_2 \le 0.5$ m, as poor on condition that 0.5 m < $H_2 \le 0.8$ m, as fair on condition that 0.8 m < $H_2 \le 1.6$ m, as good on condition that 1.6 m < $H_2 \le 5.6$ m, and as excellent on condition that $H_2 > 5.6$ m, respectively. Thus, when $0 < H_2 \le 0.7$ m, the effect of saltwater intrusion was significant, as the well water was brackish water and DWP was unacceptable to poor; when 0.7 m < $H_2 \le 0.8$ m, the effect was modest, as the well water was freshwater but DWP was poor; when $H_2 > 0.8$ m, there was no or slight effect, as the well water was freshwater and DWP was fair to excellent.

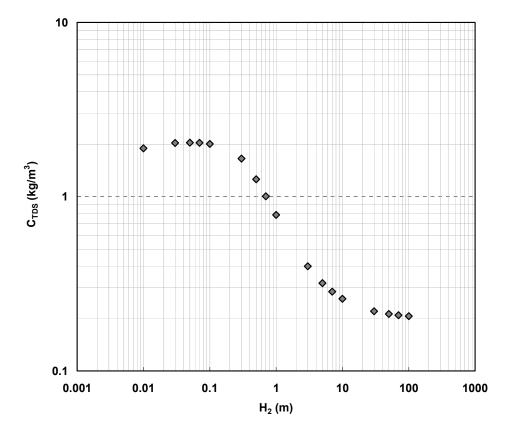


Figure 4-4 Simulations of total dissolved solids (TDS) concentration at steady-state condition in the well by hypothesis 2. The dashed line represents the concentration threshold between freshwater and brackish water.

In the case of hypothesis 2, i.e. salt diffusion through the clay, the numerical simulations demonstrated that the effect of saltwater intrusion depended on the clay thickness. According to our previous observations at the site, the clay thickness was estimated to at least 1 m. Therefore, salt diffusion through the clay with thickness greater than 1 m was not able to cause saltwater intrusion in the pumping well, which validated that hypothesis 2 could be excluded at the site.

4.4 Conclusions

In this research, it is the first time to conduct a theoretical study to test for two hypotheses about deep saline-groundwater pathways leading to saltwater upconing below a pumping well in an inland aquifer based on the field situation at the site, using a density-dependent

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groundwater flow and solute transport model. It has provided fundamental knowledge of modeling impact of deep saline-groundwater pathways on saltwater intrusion, in which the developed conceptual und numerical models as well as the key findings could enlighten to conduct further modeling studies of real field situation sharing the same or similar geological conditions.

5 Recommendations

Saltwater intrusion is a widespread contamination problem of continuing great practical interest in many coastal and inland aquifers all over the world. Therefore, it is highly desirable to properly manage groundwater resources for drinking-water supply by controlling saltwater intrusion. This paper proposes to provide two recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply at a certain waterworks site on the basis of the validated source of saltwater intrusion as well as pumping optimization, using a density-dependent groundwater flow and solute transport model. In terms of pumping-rate reduction, the optimal pumping rate was validated for eliminating the effect of saltwater intrusion. Without consideration of scenario conditions, its value could be set 1.39×10^{-2} m³/s (50 m³/h) or 5.56×10^{-3} m³/s (20 m³/h), if the requirement of drinking water palatability were good or excellent, respectively. With regard to pumping-pattern rearrangement, the well construction was modified to access bank filtration for eliminating the effect of saltwater intrusion.

Jialiang Cai, Thomas Taute, Michael Schneider

Recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply at a certain waterworks site.

Submitted to Environmental Earth Sciences (under review).

5.1 Introduction

Saltwater intrusion is a widespread problem of continuing great practical interest in many coastal and inland aquifers all over the world, which is often described by coupled density-dependent groundwater flow and advection—dispersion equations because of hydrodynamic dispersion and a wide transition zone (Bear 1972; Huyakorn and Pinder 1983; Segol 1994; Servan-Camas and Tsai 2009; Mastrocicco et al. 2012). It is considered a special category of contamination to make groundwater unsuitable for human, industry and irrigation uses, by reducing freshwater storage and in extreme cases even resulting in abandonment of drinking-water-supply wells, if salinity, generally defined as concentration of total dissolved solids (TDS), exceeds acceptable drinking water standard (El Moujabber et al. 2006; Abd-Elhamid and Javadi 2011). Therefore, it is highly desirable to properly manage groundwater resources for drinking-water supply by controlling saltwater intrusion.

In coastal aquifers, an enormous amount of studies has been conducted to control saltwater intrusion using various methods, which can be summarized as (1) reduction of pumping rates or rearrangement of pumping pattern, (2) relocation of pumping wells, (3) use of natural or artificial recharge, (4) construction of artificial subsurface barriers, (5) abstraction of saline water, and (6) combination of various techniques (Todd and Mays 2005; Abarca et al. 2006; Abd-Elhamid and Javadi 2011). Despite the fact that these aforementioned methods all have some constraints, the first alternative of pumping optimization has been proven more effective and economic using analytical or numerical models (Finney et al. 1992; Hallaji and Yazicigil 1996; Emch and Yeh 1998; Das and Datta 1999a, 1999b; Cheng et al. 2000; Gordon et al. 2000; Mantoglou 2003; Zhou et al. 2003; Abarca et al. 2006). In brief, the key issue of pumping optimization is to maintain a balance between pumping demand and quality requirements, it is thus necessary to develop appropriate models as above mentioned for determination of water quantity which can be pumped from aquifers while protecting pumping wells from saltwater intrusion

(Mantoglou 2003; Abarca et al. 2006).

With regard to inland aquifers, to our knowledge, there is greatly limited discussion for controlling saltwater intrusion to date, owing to the fact that the sources of saltwater intrusion are not routinely certain in comparison with coastal aquifers that are in hydraulic connection with the sea (Freeze and Cherry 1979; Sherif et al. 1990). Saltwater intrusion in inland aquifers may originate from various sources, including (1) seawater that entered aquifers during deposition or during a high stand of the sea in past geologic time (connate water), (2) salt in saline domes, thin beds, or disseminated in the geologic formations, (3) slightly saline water concentrated by evaporation in tidal lagoon, playas, or other enclosed areas, (4) return flows to streams from irrigated lands, and (5) anthropogenic saline wastes (Bobba 1993). Hence, it is important and essential to identify the source(s) of saltwater intrusion before implementing pumping management.

Our preliminary study (Chapter 3) has shown that is an increasingly significant effect of salinization in most abstraction wells with a great depth of ~ 50 m below the surface in an inland aguifer at the Beelitzhof waterworks (BEEWW) in southwestern Berlin (Germany) (Figure 1-1), which provides approximately 25% of total drinking-water supply for the city region. So it was assumed that the source of saltwater intrusion would originate from deeper saline groundwater. This assumption is supported by geological conditions in the Northern German Basin, where the upper fresh groundwater bearing Quaternary sediments is separated from deeper saline groundwater by Oligocene clay, whose local name in the area of Berlin is Tertiary Rupelian clay (Figure 1-2). Deep reaching Quaternary Elsterian glacial erosional channels lead to either more or less thinning of the Oligocene clay up to a complete removal. Noting that a very thin film of saline groundwater (centimeter scale) has been observed in unconsolidated fluvial fine-to-medium sandy sediments on the top of the Rupelian clay at the site, therefore, it could be assumed that Elsterian glacial channels would be in the close vicinity of the site, which results in saltwater upconing owing to pressure release by pumping a large amount of groundwater in drinking-water-production wells. Cai et al. (2014b) have tested for two hypotheses about geological conditions leading to pathways for upwelling deep saline groundwater due to pumping, which

validated that the hydraulic windows could occur in the clay caused by glacial erosion at the site and their locations under some conditions could significantly cause saltwater intrusion in the pumping well.

The principal aim of this research, consequently, was to provide recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply at BEEWW on the basis of the validated source of saltwater intrusion as well as pumping optimization, using a density-dependent groundwater flow and solute transport model. The specific objectives were to (1) reduce the pumping rate until getting the optimal value and (2) rearrange the pumping pattern by modifying the well construction for eliminating the effect of saltwater intrusion.

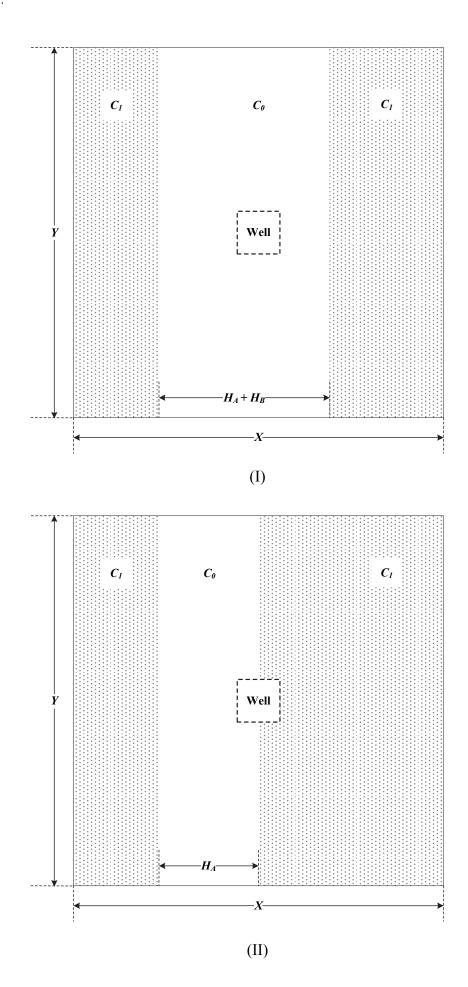
5.2 Methods

5.2.1 Conceptual model

Our preliminary study (Chapter 3) has indicated the field situation at the site in detail, which is schematically present in Figure 3-1. The conceptual model was thus accordingly developed in the lower aquifer as a confined unit, representative of the deep saline-groundwater pathway in the validated hypothesis (Figure 4-1).

Cai et al. (2014b) have demonstrated there were three scenarios of the deep saline-groundwater pathway for interpreting the validated hypothesis. They were (1) the windows A and B were located on the left- and right-hand sides of the well respectively, without consideration of H_A or H_B conditions (Scenario 1) (Figure 5-1I); (2) the window A was only located on one side of the well on condition that $H_B = 0$ (Scenario 2) (Figure 5-1II); and (3) the window A was only located on one side of the well on condition that $H_B \to +\infty$ (Scenario 3) (Figure 5-1III).

The areal effects of recharge rate (E) on the critical rise were small enough to be excluded from the analysis, according to our preliminary study (Chapter 3).



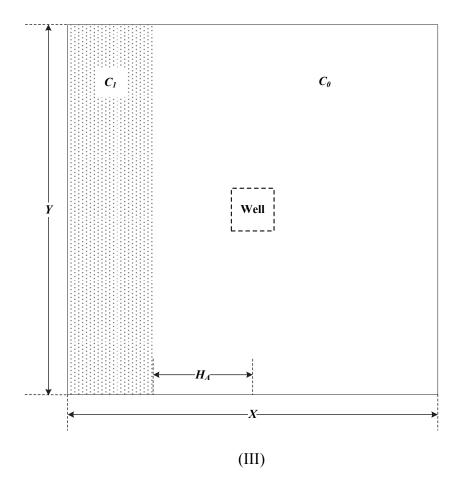


Figure 5-1 Schematic horizontal cross-section of three scenarios of the deep saline-groundwater pathway in the X-Y plane (not to scale). (I) Scenario 1: the windows A and B were located on the left- and right-hand sides of the well respectively, without consideration of H_A or H_B conditions; (II) Scenario 2: the window A was only located on one side of the well on condition that $H_B = 0$; (III) Scenario 3: the window A was only located on one side of the well on condition that $H_B \to +\infty$. C_0 and C_1 represent the total dissolved solids (TDS) concentration of fresh groundwater and saline groundwater respectively.

The areal effects of recharge rate (E) on the critical rise were small enough to be excluded from the analysis, according to our preliminary study (Chapter 3).

5.2.2 Numerical model development

Numerical modeling was performed using SEAWAT-2000 (Langevin et al. 2007). SEAWAT-2000 is a coupling of the MODFLOW groundwater flow code, modified to solve

variable-density flow conditions using equivalent freshwater head, with the MT3DMS transport model (Garabedian 2013). The coupling between fluid density and solute concentration is incorporated in the code as a linear relationship. The developed numerical model in our preliminary study (Chapter 3) was used, with specified modifications for this research.

5.2.2.1 Model discretization

The model in a two-dimensional X-Z environment was spatially discretized to form a nonuniform mesh. The columns (Δx) were variably spaced with 0.45-m horizontal resolution at the well according to the well radius (r_w) of 0.45 m at the site symmetrically expanding to 20-m horizontal resolution at the lateral boundaries (Figure 3-1). The layers (Δz) were spaced into two parts: (1) each layer was set to 10 m thick above the well screen (5 layers total); (2) each layer was set to 2 m thick below the well screen (45 layers total) (Figure 3-1). In order to minimize numerical dispersion and oscillation, the common criterion mesh Peclet number (Pe) was set to be ≤ 2 with all different Δx values (Zheng and Bennett 2002).

All simulations were performed as transient flow until steady-state conditions were reached, using the TVD advection solver, which is mass conservative, without excessive numerical dispersion and artificial oscillation (Zheng and Bennett 2002). Trial-and-error analysis demonstrated that it took 600 years to reach steady-state conditions with the current model setup, where time steps (Δt) were set to 1 year. Using this small Δt value can ensure that Courant number (Cr) correspondingly remained ≤ 1 with all different Δx values for minimization of numerical dispersion and oscillation (Zheng and Bennett 2002).

5.2.2.2 Boundary and initial conditions

The top of the model was set to no-flow boundaries according to the Holstein aquitard (Figure 3-1). The left- and right-hand sides of the model were chosen to be far enough (r_w/r_0) (the radial distance from the well center to the constant head boundary condition) =

 4.5×10^{-4}) (Figure 3-1) not to be influenced by the pumping activities (Jakovovic et al. 2011; Garabedian 2013) and implemented as 1st order boundary conditions with a constant head ($h_0 = 30$ m) and concentration ($C_0 = 0.2 \text{ kg/m}^3$) respectively. According to the observed thin film of saline groundwater in sediments on the top of the impermeable Rupelian clay, 2^{nd} order boundary conditions were chosen at the bottom of the model.

The simulated concentration was obtained at the bottom of the well screen. The concentration of saline groundwater (C_I) was incorporated as total dissolved solid (TDS) and its value was set to 5.5 kg/m³ according to the aforementioned observed thin film of saline groundwater at the site. The values of the pumping rate (Q) were varying in a range from 2.78×10^{-3} (10) to 2.78×10^{-2} m³/s (100 m³/h).

5.2.2.3 Model parameters

The model was considered to be homogeneous according to Cai et al. (2014a), with uniform parameters. The site-specified values of h_0 , hydraulic gradient (i), K_h , specific storage (S_s) and effective porosity (n_e) were measured (Table 5-1). According to our preliminary study (Chapter 3), the longitudinal (α_L) and transverse dispersivity (α_T) values were estimated to 10 and 1 m respectively. The hydraulic anisotropy (a) defined as K_h/K_v was determined to 2.3 by an integrated laboratory method called modified constant-head permeameter test (MCHPT) (Cai et al. 2014a).

5.3 Results and discussion

5.3.1 Reduction of pumping pate

5.3.1.1 Scenario 1

Table 5-1 Numerical model parameters

Para	meter	Symbol	Value	Unit
	Model width	X	2000	m
Flow Parameter	Model height	Z_3	140	m
	Initial hydraulic head	h_0	30	m
	Hydraulic gradient	i	0	-
	Horizontal hydraulic conductivity	K_h	1×10 ⁻⁴	m/s
Para	Hydraulic anisotropy	a	2.3	-
low]	Effective porosity	n_e	0.3	-
[-	Well radius	r_w	0.45	m
	Length of well screen	L_{ws}	30	m
	D	Q	2.78×10^{-3} , 1.11×10^{-2} ,	3,
	Pumping rate		1.94×10 ⁻² , 2.78×10 ⁻²	m^3/s
	Specific storage	S_s	5×10 ⁻⁴	1/m
	Longitudinal dispersivity	Z_3 Z_3 Z_4 Z_5 Z_5 Z_6 Z_7 Z_8	10	m
eter	Transverse dispersivity	α_T	1	m
ram	Effective diffusion coefficient in porous media	D^*	1×10 ⁻¹⁰	m^2/s
rt Pa	Total dissolved solids (TDS) concentration of	C	0.2	kg/m ³
Transport Parameter	fresh groundwater	C_0	0.2	
Tra	TDS concentration of saline groundwater	C_{I}	5.5	kg/m ³
	Lateral distance from the well to windows	7.7	0. 1000	
	in the Rupelian clay	Н	0~1000	m

When $Q = 2.78 \times 10^{-2}$ m³/s (100 m³/h), the salinity in the well was estimated to be 1 kg/m³ when $H_A + H_B = 1100$ m (regression equation not shown, the same as blow) (Figure 5-2I), i.e. the well water was classified as brackish water on condition that $0 < H_A + H_B \le 1100$ m, noting the criteria listed in Table 3-2. Owing to the fact that our recommendations aimed to control saltwater intrusion for drinking-water supply at BEEWW, it was thus essential to

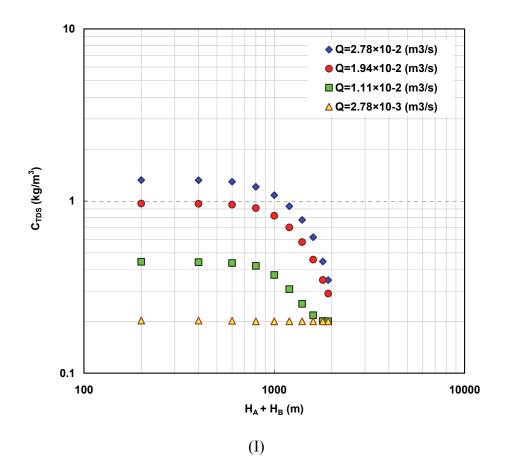
consider the impact of TDS concentration on drinking water palatability (DWP) as well. According to the criteria listed in Table 4-2, DWP was classified as unacceptable on condition that $0 < H_A + H_B \le 800$ m, as poor on condition that 800 m $< H_A + H_B \le 1230$ m, as fair on condition that 1230 m $< H_A + H_B \le 1610$ m, and as good on condition that 1610 m $< H_A + H_B \le 1920$ m, respectively. Therefore, when $0 < H_A + H_B \le 1100$ m, the effect of saltwater intrusion was significant, as the well water was brackish water and DWP was unacceptable to poor; when 1100 m $< H_A + H_B \le 1230$ m, the effect was modest, as the well water was freshwater but DWP was poor; when 1230 m $< H_A + H_B \le 1920$ m, there was no or slight effect, as the well water was freshwater and DWP was fair to good.

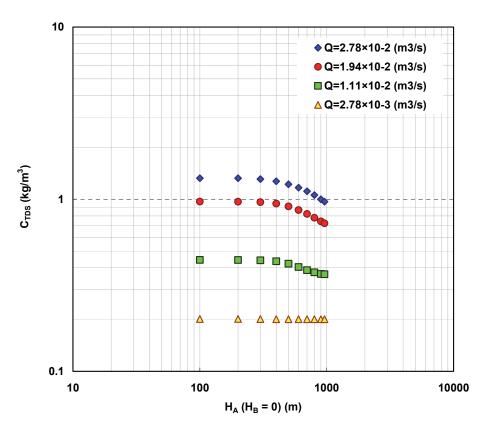
When $Q = 1.94 \times 10^{-2}$ m³/s (70 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2I). DWP was classified as poor on condition that $0 < H_A + H_B \le 820$ m, as fair on condition that $820 < H_A + H_B \le 1360$ m, as good on condition that 1360 m $< H_A + H_B \le 1900$ m, and as excellent on condition that 1900 m $< H_A + H_B \le 1920$ m, respectively. Thus, when 0 m $< H_A + H_B \le 820$ m, the effect of saltwater intrusion was modest; when 820 m $< H_A + H_B \le 1920$ m, there was no or slight effect.

When $Q = 1.11 \times 10^{-2}$ m³/s (40 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2I). DWP was classified as good on condition that $0 < H_A + H_B \le 1220$ m, and as excellent on condition that 1220 m $< H_A + H_B \le 1920$ m, respectively. Therefore, there was no effect of saltwater intrusion.

When $Q = 2.78 \times 10^{-3}$ m³/s (10 m³/h), the salinity of all simulations was almost as identical as C_0 , so no saltwater upconing occurred (Figure 5-2I).

Consequently, according to the correlation of the salinity in the well to Q on condition that $H_A + H_B = 200$ m (Figure 5-3), it could be estimated in all simulations that there was no effect of saltwater intrusion and DWP was good when $Q = 1.39 \times 10^{-2}$ m³/s (50 m³/h) as well as DWP was excellent when $Q = 5.56 \times 10^{-3}$ m³/s (20 m³/h).





(II)

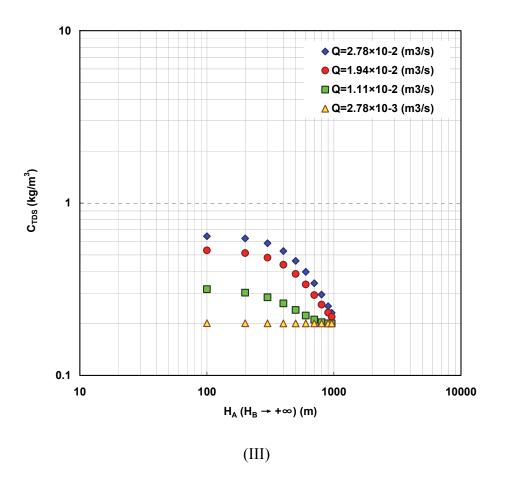


Figure 5-2 Simulations of total dissolved solids (TDS) concentration at steady-state condition in the well with varying pumping rate (Q) by Scenario 1 (I), Scenario 2 (II), and Scenario 3 (III), respectively. The dashed line represents the concentration threshold between freshwater and brackish water.

5.3.1.2 Scenario 2

When $Q = 2.78 \times 10^{-2}$ m³/s (100 m³/h), the salinity in the well was estimated to be 1 kg/m³ when $H_A = 865$ m (Figure 5-2II), i.e. the well water was classified as brackish water on condition that $0 < H_A \le 865$ m. DWP was classified as unacceptable on condition that $0 < H_A \le 530$ m, and as poor on condition that 530 m $< H_A \le 960$ m, respectively. Thus, when $0 < H_A \le 865$ m, the effect of saltwater intrusion was significant; when 865 m $< H_A \le 960$ m, the effect was modest.

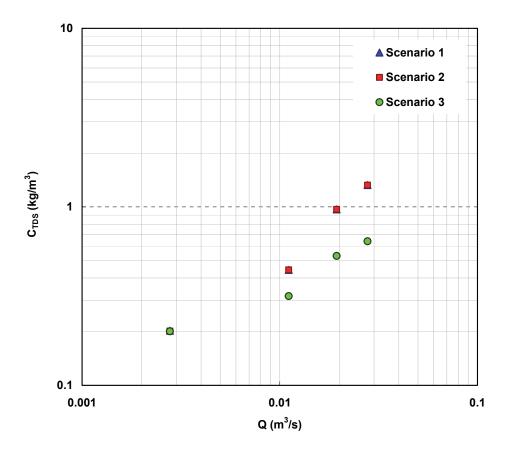


Figure 5-3 Correlation of total dissolved solids (TDS) concentration at steady-state condition in the well to pumping rate (Q) in Scenario 1 on condition that $H_A + H_B = 200$ m, Scenario 2 on condition that $H_A = 100$ m, and Scenario 3 on condition that $H_A = 100$ m, respectively. The dashed line represents the concentration threshold between freshwater and brackish water.

When $Q = 1.94 \times 10^{-2}$ m³/s (70 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2II). DWP was classified as poor on condition that $0 < H_A \le 520$ m, as fair on condition that 520 m $< H_A \le 960$ m, respectively. Therefore, when 0 m $< H_A \le 520$ m, the effect of saltwater intrusion was modest; when 520 m $< H_A \le 960$ m, the effect was slight.

When $Q = 1.11 \times 10^{-2}$ m³/s (40 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2II). DWP of all simulations was classified as good. Thus, there was no effect of saltwater intrusion.

When $Q = 2.78 \times 10^{-3} \text{ m}^3/\text{s}$ (10 m³/h), the salinity of all simulations was almost as identical as C_0 , so no saltwater upconing occurred (Figure 5-2II).

Consequently, according to the correlation of the salinity in the well to Q on condition that $H_A = 100$ m (Figure 5-3), it could be estimated in all simulations that there was no effect of saltwater intrusion and DWP was good when $Q = 1.39 \times 10^{-2}$ m³/s (50 m³/h) as well as DWP was excellent when $Q = 5.56 \times 10^{-3}$ m³/s (20 m³/h), the same as Scenario 1.

5.3.1.3 Scenario 3

When $Q = 2.78 \times 10^{-2}$ m³/s (100 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2III). DWP was classified as fair on condition that $0 < H_A \le 265$ m, as good on condition that 265 m $< H_A \le 790$ m, and as excellent on condition that 790 m $< H_A \le 960$ m, respectively. Therefore, there was no or slight effect of saltwater intrusion.

When $Q = 1.94 \times 10^{-2}$ m³/s (70 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2III). DWP was classified as good on condition that $0 < H_A \le 685$ m, as excellent on condition that 685 m $< H_A \le 960$ m, respectively. Thus, there was no effect of saltwater intrusion.

When $Q = 1.11 \times 10^{-2}$ m³/s (40 m³/h), the well water of all simulations was classified as freshwater (Figure 5-2III). DWP was classified as good on condition that $0 < H_A \le 210$ m, as excellent on condition that 210 m $< H_A \le 960$ m, respectively. Therefore, there was no effect of saltwater intrusion.

When $Q = 2.78 \times 10^{-3} \text{ m}^3/\text{s}$ (10 m³/h), the salinity of all simulations was as identical as C_0 , so no saltwater upconing occurred (Figure 5-2III).

Consequently, according to the correlation of the salinity in the well to Q on condition that $H_A = 100$ m (Figure 5-3), it could be estimated in all simulations that there was no effect of saltwater intrusion and DWP was good when $Q = 2.50 \times 10^{-2}$ m³/s (90 m³/h) as well as DWP was excellent when $Q = 8.34 \times 10^{-3}$ m³/s (30 m³/h).

Overall, the optimal $Q(Q_{opt})$ was validated for eliminating the effect of saltwater intrusion at BEEWW. Without consideration of scenario conditions, its value could be set 1.39×10^{-2} m³/s (50 m³/h) or 5.56×10^{-3} m³/s (20 m³/h), if the requirement of DWP were good or excellent, respectively.

5.3.2 Modification of well construction

As noted, the key issue of pumping optimization is to maintain a balance between pumping demand and drinking-water quality requirements. However, the aforementioned Q_{opt} with a value of 5.56×10^{-3} m³/s (20 m³/h) would be apparently a low pumping rate, if the requirement of DWP were excellent, which would hardly meet the demand of drinking-water supply for cities like Berlin. Thus, it was necessary to rearrange the pumping pattern by modifying the well construction for controlling saltwater intrusion, while maintaining the present pumping rate, e.g. $Q = 2.78\times10^{-2}$ m³/s (100 m³/h).

The Friedrichshagen waterworks (FRIWW) is located in southeastern Berlin (Figure 1-1), which shares the same geological conditions as BEEWW. However, no effect of saltwater intrusion has been observed in pumping wells with a depth of 50 m below the surface at FRIWW, owing to the fact that there is no aquitard dividing the fresh groundwater aquifer. Therefore, the bank filtration from Lake Müggelsee to pumping wells occurs to play an important role for controlling saltwater intrusion. Hass (2012) showed that there is approximately 70% bank filtration for total drinking-water supply at FRIWW. Hence, the well screen could be built in the upper aquifer to access bank filtration from Lake Wannsee for eliminating the effect of saltwater intrusion at BEEWW (Figure 5-4). Based on the situation at FRIWW, there was no need to conduct further numerical modeling to validate the effect of the well-construction modification.

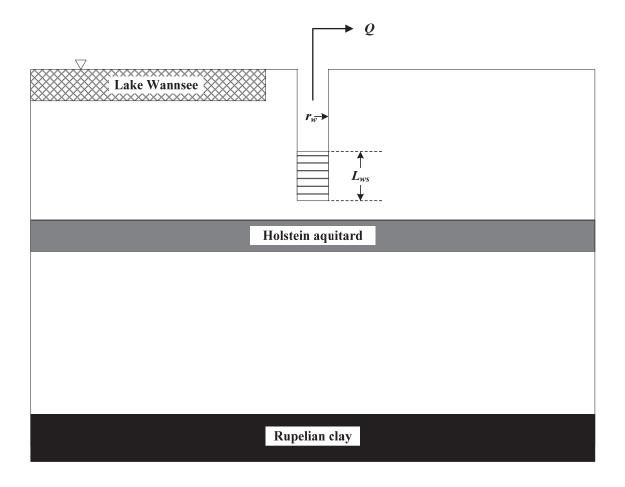


Figure 5-4 Schematic vertical cross-section of well-construction modification (not to scale). L_{ws} - length of well screen; r_w - well radius; Q - pumping rate.

5.4 Summary and conclusions

This research provided two recommendations of controlling saltwater intrusion in an inland aquifer for drinking-water supply at BEEWW in southwestern Berlin (Germany) on the basis of the validated source of saltwater intrusion as well as pumping optimization, using a density-dependent groundwater flow and solute transport model. The key findings are summarized as follows:

• In terms of pumping-rate reduction, Q_{opt} was validated for eliminating the effect of saltwater intrusion. Without consideration of scenario conditions, its value could be set 1.39×10^{-2} m³/s (50 m³/h) or 5.56×10^{-3} m³/s (20 m³/h), if the requirement of DWP were good or excellent, respectively. It was demonstrated an effective and economic

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measure for controlling saltwater intrusion, but might hardly meet the demand of drinking-water supply due to its strict quality requirements.

• In terms of pumping-pattern rearrangement, the well construction was modified to access bank filtration for eliminating the effect of saltwater intrusion by building the well screen in the upper aquifer. It was demonstrated an effective measure for controlling saltwater intrusion while maintaining the present pumping rate, but would require financial investments in advance.

6 Conclusions

6.1 Major outcomes

This thesis has conducted an integrated study of hydraulic anisotropy and its impact on saltwater intrusion in an inland aquifer at the Beelitzhof waterworks (BEEWW) in southwestern Berlin (Germany), which includes (1) establishing a new laboratory method for the efficient determination and verification of consistent values of directional hydraulic conductivity (DHC) in fine-to-medium sandy sediments, (2) modeling the impact of hydraulic anisotropy (*a*) as well as deep saline-groundwater sources on saltwater intrusion due to pumping, and (3) providing recommendations of controlling saltwater intrusion for drinking-water supply.

The major outcomes of each core chapter are respectively summarized as follows:

Chapter 2: Laboratory method

- Undisturbed 25-cm core samples (25CS) and 6.5-cm core samples (6.5CS) were obtained for measuring vertical and horizontal hydraulic conductivity (K_{ν} and K_h) respectively by a newly developed method. The integrity of the 6.5CS samples from the 25CS samples was validated by bulk density (ρ_b), which indicated that the differences between the $\rho_{b_{6.5CS}}$ value and the average value of two $\rho_{b_{25CS}}$ values were < 1%.
- A precise and standardized procedure for preparing the experimental setup of modified constant-head permeameter test (MCHPT) was conducted based on an integrated experimental setup of constant-head permeameter test and tracer tests by modifying the outer tubing diameter of 8 mm and the tracer injection point for the valid applicability of the Darcy equation. Moreover, a formula (Equation 2-9) was provided for the time-optimized control of sample saturation.
- The determination of K_h and K_v values showed that all the K_h values were on average ~2.3 times greater than the K_v values, and both of them were greater than 1.7×10^{-6}

- m/s (K_{min}) but less than the K value of the experimental setup (K_{setup}). They were validated by tracer tests with effective porosity (n_e) < 0.5.
- In comparison with grain size-based methods, the validity of consistent K_h and K_v values determined by MCHPT was convincing.
- An efficient, precise, and applicable methodological framework of MCHPT for the general determination and verification of DHC values in fine-to-medium sandy sediments can be obtained for further investigation (Figure 2-12).

Chapter 3: Modeling study I

Impact of hydraulic anisotropy on saltwater intrusion

- A conceptual model representative of the field situation was developed and implemented in a numerical density-dependent groundwater flow and solute transport model.
- The uncertain values of longitudinal and transverse dispersivity were estimated to 10 and 1 m respectively, according to the assessment of their impacts on saltwater intrusion.
- The impact of *a* on saltwater intrusion was validated to be not significant due to the hydrogeological conditions at the site, based on its precise value of 2.3 in comparison with the empirical value of 10.

Chapter 4: Modeling study II

Impact of deep saline-groundwater sources on saltwater intrusion

- Hypothesis 1, defined as there are hydraulic windows in the Rupelian clay caused by glacial erosion, where their locations are uncertain, was validated with 4 scenarios that windows could occur in the clay at the site and their locations under some conditions could significantly cause saltwater intrusion.
- Hypothesis 2, defined as there are no windows in the clay, but the clay is partially
 thinned out but not completely removed by glacial erosion, so salt can merely come
 through the clay upwards by diffusion and eventually accumulate on its top, could be

excluded, because salt diffusion through the clay with thickness greater than 1 m at the site was not able to cause saltwater intrusion.

Chapter 5: Recommendations

- In terms of pumping-rate reduction, the optimal pumping rate was validated for eliminating the effect of saltwater intrusion. Without consideration of scenario conditions, its value could be set 1.39×10^{-2} m³/s (50 m³/h) or 5.56×10^{-3} m³/s (20 m³/h), if the requirement of drinking water palatability were good or excellent, respectively. It was demonstrated an effective and economic measure for controlling saltwater intrusion, but might hardly meet the demand of drinking-water supply due to its strict quality requirements.
- In terms of pumping-pattern rearrangement, the well construction was modified to access bank filtration for eliminating the effect of saltwater intrusion by building the well screen in the upper aquifer. It was demonstrated an effective measure for controlling saltwater intrusion while maintaining the present pumping rate, but would require financial investments in advance.

Overall, the highlights of this thesis can be summarized as follows:

- It is the first time to efficiently determine and verify precise consistent DHC values in fine-to-medium sandy sediments by developing an integrated laboratory method called MCHPT.
- It is the first time to identify deep saline-groundwater sources in an inland aquifer and validate their impacts on saltwater intrusion by testing for two hypotheses about geological conditions leading to pathways for upwelling deep saline groundwater due to pumping, using a density-dependent groundwater flow and solute transport model.

6.2 Outlook

This thesis has provided fundamental knowledge of modeling impact of deep

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saline-groundwater sources on saltwater intrusion in an inland aquifer and correspondingly recommending some appropriate measures of groundwater resources management by controlling saltwater intrusion for drinking-water supply at a certain waterworks site.

Owing to the fact that the theoretical modeling study conducted in this thesis was simplified into a two-dimensional environment (vertical cross-section) with a pumping well, the following suggestions could therefore arise for the future research.

- To conduct a three-dimensional analysis for deepening the obtained fundamental knowledge in order to more accurately simulate the field situation.
- To expand the modeling study with two pumping wells, multiple pumping wells, till an entire well gallery at the site in order to more accurately simulate the field situation. Accordingly, the pumping pattern could be rearranged to coordinate the pumping interaction between the wells for controlling saltwater intrusion.
- To further develop new methods that are more effective and economic than pumping optimization for controlling saltwater intrusion.

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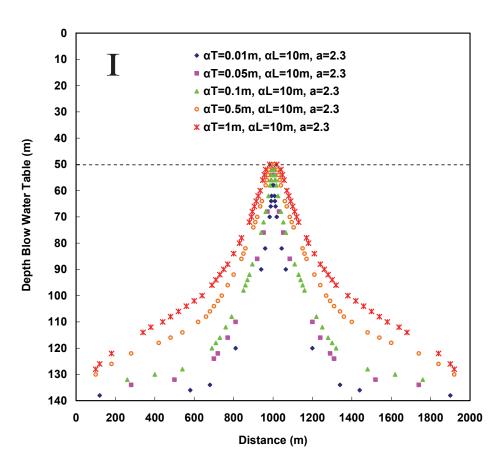
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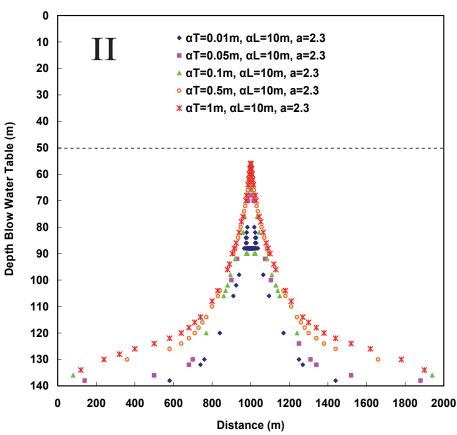
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Appendix

Appendix I – Figures





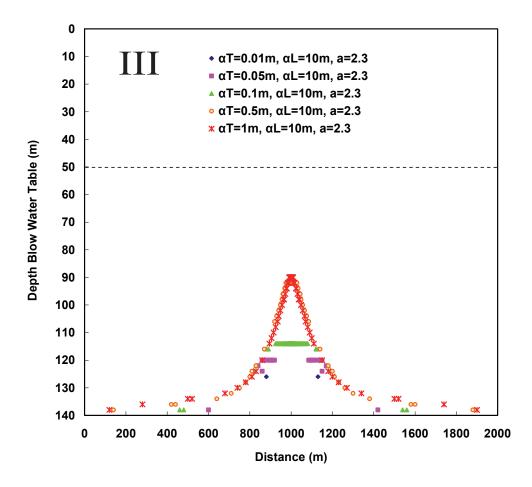
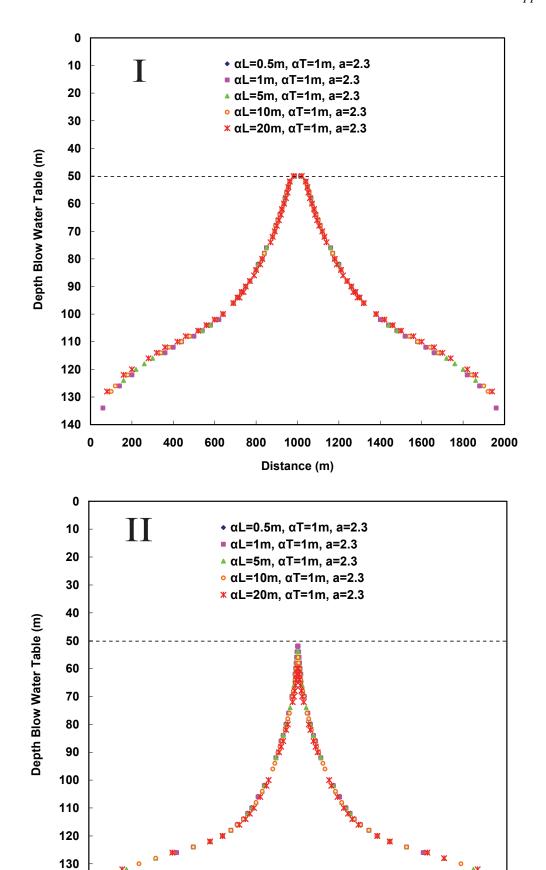


Figure A-1 Saltwater upconing distribution at steady-state condition with varying transverse dispersivity (α_T) by 20% (I), 50% (II), and 80% (III) contour of total dissolved solids (TDS) concentration respectively. (1) Longitudinal dispersivity (α_L) and hydraulic anisotropy (a) were set to constant values of 10 m and 2.3 respectively; (2) the dashed line represents the bottom of the well screen.



140 ^L

Distance (m)

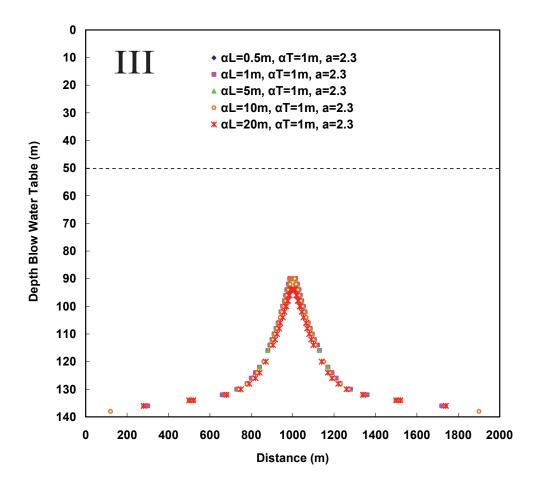
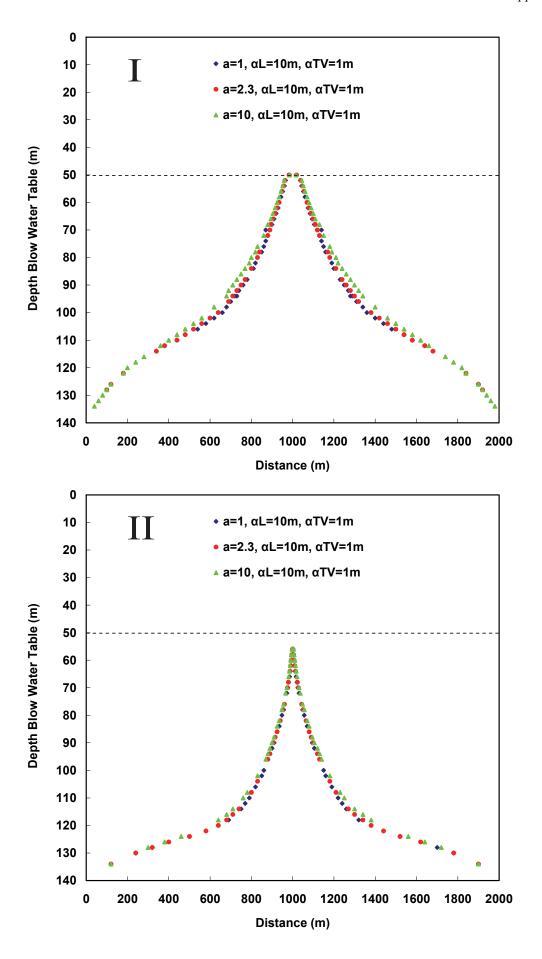


Figure A-2 Saltwater upconing distribution at steady-state condition with varying longitudinal dispersivity (α_L) by 20% (I), 50% (II), and 80% (III) contour of total dissolved solids (TDS) concentration respectively. (1) Transverse dispersivity (α_T) and hydraulic anisotropy (a) were set to constant values of 1 m and 2.3 respectively; (2) the dashed line represents the bottom of the well screen.



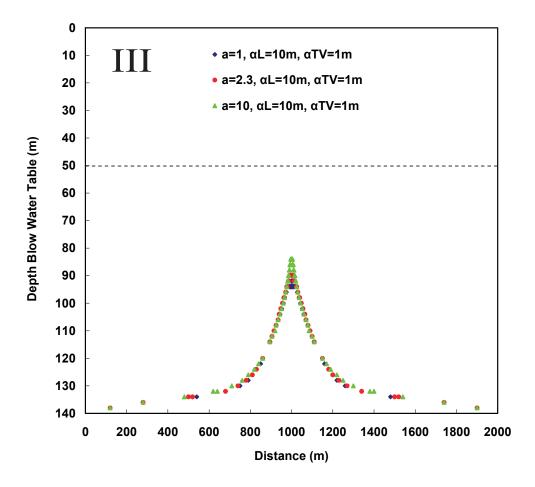


Figure A-3 Saltwater upconing distribution at steady-state condition with varying hydraulic anisotropy (a) by 20% (I), 50% (II), and 80% (III) contour of total dissolved solids (TDS) concentration respectively. (1) Longitudinal dispersivity (α_L) and transverse dispersivity (α_T) were set to constant values of 10 m and 1 m respectively; (2) the dashed line represents the bottom of the well screen.

Appendix II – List of publications

INTERNATIONAL PEER-REVIEWED JOURNAL ARTICLES

Cai, J., Taute, T., Schneider, M.: Recommendations of Controlling Saltwater Intrusion in an Inland Aquifer for Drinking-Water Supply at a Certain Waterworks Site. *Environmental Earth Sciences*. (under review)

Cai, J., Taute, T., Schneider, M.: A Theoretical Modeling Study on Impact of Hydraulic Anisotropy on Saltwater Intrusion in a Pumping Well in an Inland Aquifer. *Environmental and Engineering Geoscience*. (under review)

Cai, J., Taute, T., Schneider, M., 2014. Saltwater Upconing Below a Pumping Well in an Inland Aquifer: A Theoretical Modeling Study on Testing Different Scenarios of Deep Saline-Groundwater Pathways. *Water*, *Air*, & *Soil Pollution*. http://dx.doi.org/10.1007/s11270-014-2203-7.

Cai, J., Taute, T., Hamann, E., Schneider, M., 2014. An Integrated Laboratory Method to Measure and Verify Directional Hydraulic Conductivity in Fine-to-Medium Sandy Sediments. *Groundwater*. http://dx.doi.org/10.1111/gwat.12156.

Huang, Y., Wen, H., Cai, J., Cai, M., Sun, J., 2010. Key Aquatic Environmental Factors Affecting Ecosystem Health of Streams in the Dianchi Lake Watershed, China. *Procedia Environmental Sciences*, (2), 868–880.

Huang, Y., Cai, J., Yin, H., Cai, M., 2009. Correlation of Precipitation to Temperature Variation in the Huanghe River (Yellow River) Basin during 1957-2006. *Journal of Hydrology*, 372(1-4), 1-8.

CHINESE PEER-REVIEWED JOURNAL ARTICLES (with English abstract)

Cai, J., Su, Y., Wen, H., Wang, D., Huang, Y., 2011. Characteristics of Macrozoobenthic Assemblages and their Relationship with Aquatic Environmental Factors in Streams of Lake Dianchi Watershed in the Wet Season. *Journal of Environmental Sciences*, 32(4), 982-989.

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