Solute transport in heterogeneous aquifers
parameter identification and its use in groundwater pollution and
salt water intrusion problems

Opgeloste stoffen transport in heterogene grondwaterreservoirs
parameteridentificatie en het gebruik hiervan in grondwaterverontreinigings- en
zoutwaterintrusieproblematiek

Alexander Vandenbohede

Promotor: Prof. Dr. L. Lebbe

Proefschrift voorgelegd tot het behalen van de graad van Doctor in de Wetenschappen,
richting Geologie
Table of contents

Acknowledgements

Publications

Chapter 1: Introduction

1.1 The earth: a thirsty planet 1
1.2 Focus on solute transport 3
1.3 Structure of the dissertation 5

Chapter 2: On Groundwater Flow, Solute Transport and Parameter Identification Tests

2.1 Groundwater flow 7
  2.1.1 Darcy’s law 7
  2.1.2 Groundwater flow equation 9
2.2 Solute transport 12
2.3 Diffusion and mechanical dispersion 13
  2.3.1 Diffusion 13
  2.3.2 Mechanical dispersion 15
2.4 Dispersion coefficient on microscopic scale 15
2.5 Derivation of the Advection-Dispersion Equation (ADE) for solute transport 17
  2.5.1 Derivation of the ADE 17
  2.5.2 Hydrodynamic dispersion 19
2.6 Parameter identification 20
  2.6.1 Introduction 20
  2.6.2 Hydraulic parameter identification tests 20
  2.6.3 Solute transport parameter identification tests 23

Chapter 3: Aquifer Heterogeneity

Effects on hydraulic and solute transport parameters

3.1 Heterogeneity of groundwater reservoirs 24
3.2 Hydraulic parameters in heterogeneous aquifers 25
  3.2.1 Hydraulic conductivity 25
  3.2.2 Specific elastic storage 26
3.3 Solute transport parameters in heterogeneous aquifers 27
  3.3.1 Dispersivity 28
  3.3.2 Porosity 31
Chapter 4: Parameter Identification tests

Development of usable tests

4.1 Selection of an appropriate test
   4.1.1 Introduction
   4.1.2 Forced gradient tracer test
   4.1.3 Type of tracer and method of observation
   4.1.4 EM39 conductivity and total dissolved solids

4.2 Pumping test analyses
   4.2.1 Analytical solutions
   4.2.2 HYPARIDEN: a model package for pumping test analyses

4.3 TRACER3D: numerical model for tracer test analyses
   4.3.1 TRACER3D program package
      4.3.1.1 Calculation of advection and dispersion
      4.3.1.2 Stability criteria
      4.3.1.3 Calculation of observations
      4.3.1.4 Simulation of injection
   4.3.2 Validation of TRACER3D

4.4 Conformity between tracer and pumping tests
4.5 Derivation of chemical parameters
   4.5.1 Push-pull test: concepts
   4.5.2 In situ determination of reaction rate coefficients

Chapter 5: To the field

Parameter identification tests in practice

5.1 Introduction
5.2 Houtave test site: proof of concept
   5.2.1 Introduction
   5.2.2 (Hydro)geological site characterisation
   5.2.3 Pumping test
   5.2.4 Forced gradient tracer test
      5.2.4.1 Presentation of observations and qualitative analyses
      5.2.4.2 Interpretation with an analytical model
      5.2.4.3 Analytical pumping test interpretation
      5.2.4.4 Dispersivity values from the tracer test
   5.2.5 3D simulation with TRACER3D
   5.2.6 Sensitivity analyses
   5.2.7 Identification of transverse dispersivity
   5.2.8 General discussion and conclusions on the Houtave test site
5.3 Zevergem test site
   5.3.1 Introduction
   5.3.2 (Hydro)geological site characterisation
   5.3.3 Pumping test
   5.3.4 Double forced gradient tracer test
      5.3.4.1 Presentation of observations and qualitative analyses
      5.3.4.2 Interpretation with TRACER3D
   5.3.5 Discussion and conclusions
5.4 Tessenderlo test site: to an application
   5.4.1 Introduction
   5.4.2 Step drawdown test
5.4.3 Forced gradient tracer test 99
5.4.4 Modelling the injection phase and the solute balance 104
5.4.5 Discussion and conclusions 106
5.5 Injection of the tracer 106
5.6 Push-pull tests 108
  5.6.1 Introduction 108
  5.6.2 Pus-pull test on the Houtave test site 108
5.7 Discussion and conclusions of the field tests 115
  5.7.1 Forced gradient tracer test 115
  5.7.2 Push-pull test 119

Chapter 6: Effects of Aquifer Heterogeneity on Pumping Tests

6.1 Introduction 121
6.2 Groundwater flow model RMOQ3D 122
  6.2.1 General introduction 122
  6.2.2 Simulation of pumping tests in a homogeneous aquifer 122
  6.2.3 Simulation of pumping tests in a heterogeneous aquifer 124
6.3 Field example 128

Chapter 7: Applications of Field Derived Parameters
Models as a synthesis of available knowledge

7.1 Introduction 131
7.2 Field scale applications 131
  7.2.1 Introduction 131
  7.2.2 Case study: Tessenderlo test site 132
    7.2.2.1 Introduction 132
    7.2.2.2 Towards a remediation scheme 133
    7.2.2.3 Conclusions 135
7.3 Regional scale applications 135
  7.3.1 Regional groundwater flow models 135
  7.3.2 Case study: Houtave channel ridge 140
    7.3.2.1 Introduction 140
    7.3.2.2 Geological history 140
    7.3.2.3 Study area 143
    7.3.2.4 Methodology 144
    7.3.2.5 Water quality analyses 146
    7.3.2.6 Numerical model of the inverted channel ridge 148
    7.3.2.7 Sensitivity analyses 150
    7.3.2.8 Conclusions 152
  7.3.3 Case study: The ‘Westhoek’ nature reserve 152
    7.3.3.1 Introduction 152
    7.3.3.2 Evolution in time of the flow system 160
    7.3.3.3 Sensitivity analyses 162
    7.3.3.4 Influence of tides 164
    7.3.3.5 Effects of storms 168
    7.3.3.6 Influence of monthly infiltration variations 173
    7.3.3.7 Future sea level change and changes in coastal morphology 175
    7.3.3.8 Conclusions 189
Chapter 8: Conclusions and Final Remarks

8.1 Introduction 191
8.2 Parameter identification tests 192
   8.2.1 Forced gradient tracer test 192
   8.2.2 Collection of the observations 193
   8.2.3 Interpretation of the forced gradient tracer test 193
   8.2.4 Applications: Houtave, Zevergem and Tessenderlo test sites 194
   8.2.5 Results of the forced gradient tracer tests 194
   8.2.6 Longitudinal dispersivity 195
   8.2.7 Influence of heterogeneity on pumping test results 197
   8.2.8 Push-pull test 197
8.3 Applications of parameter identification tests 198
   8.3.1 Applications on field scale: groundwater pollution problems 198
   8.3.2 Regional groundwater flow models 198
   8.3.3 Case study: the Stalhille channel ridge 199
   8.3.4 Case study: Westhoek nature reserve 200

Samenvatting 203

References 217
On the morning of 31 May 2003 the sun rose partially eclipsed above the mist shrouded polder landscape of the Nieuwe Polder van Blankenberge (A. Vandenbohede).
This dissertation is the result of nearly 5 years of research at the Department of Geology and Soil Science of Ghent University. Obviously, finishing this Ph.D. research was not my merit alone. Above all, I would like to express my sincere appreciation to my promoter, Prof. Dr. L. Lebbe. He provided the opportunity to start this research and to keep it going. His enthusiasm about hydrogeology in general and hydrology and geology of the coastal plain are inspiring. Thanks Luc for given me the freedom to explore the topics I was interested in.

I thank F. Fynn, M. Genbrugge, E. Pauwels and R. Bogaert for their enthusiastic help during parts of my field work. Discussions with Ir. E. Beeuwsaert about the practical side of field work and the design of all sorts of attributes to measure all sorts of things were always enlightening. I could count on J. Beeckman, with a joke in between of course, for explanations on water analyses and laboratory procedures. Thank you guys from the labs.

Fieldwork forms an important part of hydrogeological and geological research. Therefore, I express my gratitude to the landowners who led us use their land to do drillings, install wells and perform field tests. I also thank T. Claes for sharing data on the Tessenderlo field site and for his aid during the field work.

I would like to thank prof. dr. ir. W. Verstraete and dr. ir. S. De Wildeman of the Laboratory for Microbial Ecology and Technology (LabMET) of Ghent University. They introduced me in the ever fascinating world of microbiology.

Appreciation goes to my colleges at the department of geology and soil science, some already long gone: Dr. A. Chaouni Alia, Dr. N. El Halimi, R. Eppinger, J. Lermytte, Drs. A. Louwyck, D. Vandevelde, Dr. N. Van Meir. Discussions on hydrogeology and research in general were very helpful seeing things in perspective.

During this research I was working as academic assistant in the Department of Geology and Soil Science of Ghent University. My gratitude goes to the staff of the department to give me this opportunity. I would like to thank specifically Prof. Dr. J.-P. Henriet, Prof. Dr. P. Jacobs, Prof. Dr. R. Nijs and Prof. Dr. G. Stoops with whom it was pleasant and interesting working during practical exercises, lessons and excursions. My work as assistant definitely broadened my view as a geologist.

Part of this dissertation is already published. Therefore, I would like to thank the reviewers giving valuable comments on the publications and providing feed-back during the research for this dissertation: Dr. H. Kooi (Free University Amsterdam, Faculty of Earth and Life Science), Dr. Ir. G.H.P. Oude Essink (Free University Amsterdam, Faculty of Earth and Life Science), Dr. V. Post (Free University Amsterdam, Faculty of Earth and Life Science), Prof. Dr. K. Thorbjarnarson (San Diego State University, Department of Geological Sciences) and some anonymous reviewers.

The acknowledgement is perhaps the only part that will be read by anyone looking into this dissertation. Therefore, I sincerely hope I did not forget someone. I’m the only one to blame if so.
Part of this work has already been published:


Chapter 1

Introduction

We cannot understand the consultants who rarely model (Bredehoeft & Hall, 1995)

1.1 The earth: a thirsty planet

When you read this dissertation, 1.75 million people will have died before their time in the past year because they have no access to safe drinking water. It is the toll from cholera, dysentery and other diarrhoeal diseases that the World Health Organisation attributes to unsafe drinking supplies.

The type of water we generally use in human activities is fresh water. However, only 4.9% of the world's water supply is fresh water. One-third of that is frozen forming the polar ice caps, glaciers, and icebergs. The rest of the total fresh water supply is available as either surface water or groundwater. Considering an average sized bath-tube, the available water to man is than only filling a little spoon. Groundwater accounts here for the most important supply. These figures show the importance of groundwater to current society. Usage of this supply is tripled in the last 50 years. Agriculture (75%), industry (20%) and domestic purposes (5%) are on a global scale the most important users. To raise awareness and galvanise action to better manage and protect the crucial water resources, the United Nations General Assembly proclaimed 2003 as the International Year of Freshwater (Water Year 2003). Two critical areas are considered. The first is the already mentioned degradation of water quality causing water-borne diseases. The other area is water stress and scarcity.

![Distribution of Earth’s water storages.](source: Adapted from Figure 2. Freshwater Series No. A-2, “Water — Here, There and Everywhere”)

A 2002 United Nations rapport ‘Vital Water Graphics’ from the United Nations Environment Programme (UNEP) has taken together statistics and data on past and current water use and supplies and extrapolated these, taken into account future growth of the world’s population. The picture resulting from this report is quite bleak. It is estimated that two-thirds of the world’s population are destined to be living in water stressed areas. An area is experiencing water stress when annual water supplies drop below 1700 m³ per person. When annual water supplies drop below 1000 m³ per person, the population faces water scarcity. Water scarcity occurs when the amount of water withdrawn from lakes, rivers or groundwater is so large that water supplies are no longer adequate to satisfy all human
or ecosystem requirements, resulting in increased competition between water users and demands. Some 460 million people - more than 8% of the world’s population - live in countries using so much of their freshwater resources that they can be considered highly water stressed (UNCSD, 1999; WMO 1997). A further 25% of the population lives in countries approaching a position of serious water stress (WMO, 1997). According to Population Action International, based upon the UN Medium Population Projections of 1998, more than 2.8 milliard people in 48 countries will face water stress or scarcity conditions by 2025. Of these countries, 40 are in West Asia, North Africa or Sub-Saharan Africa. Over the next two decades, population increases and growing demands are projected to push all the West Asian countries into water scarcity conditions. By 2050, the number of countries facing water stress or scarcity could rise to 54, with their combined population being 4 milliard people - about 40% of the projected global population of 9.4 milliard (Gardner-Outlaw and Engleman, 1997; UNFPA, 1997). Heating up of the earth, global change and its consequences may be the most important global challenges of the future, water scarcity and quality degradation are a very close second and are of course highly related to it.

![Figure 1.2 Global freshwater stress in 1995 and projections into the future.](image)

But it is at the political level that the battle to avert a global water crisis will ultimately be won or lost. One of the issues in this context is privatisation of water supplies. The danger exists that safe water is degraded to no more than merchandise for which hard cash must be paid leaving the poorest to contaminated rivers or wells for their supplies. Dramatic examples of this in for instance South-Africa and Ghana are already happening.

The focus is not only on Asia or Africa. Belgium is, very oddly, bottom of the world rankings for water quality in a UN World Water Development Report released in 2003. Is it then safer to drink tap water in for instance Ghana than in Brussels? Of course not but it is argued that various aspects of water resources management must be taken into account. Heavy industrial pollution and agricultural run-off, compounded with inadequate wastewater treatment and balkanised government responsibility for the issue explain Belgium’s position. Albeit, it is a firm signal to policy makers to promote a more integrated water management on different levels.

An important issue in groundwater quality and supply degradation is groundwater contamination. It occurs when man-made products such as gasoline, oil, chemicals, etc. get into the groundwater and...
cause it to become unsafe and unfit for human use. Some of the major sources of these products, called contaminants, are storage tanks, septic systems, hazardous waste sites, landfills, and the widespread use of chemicals. Another pressing issue is seawater or salt water intrusion. Due to natural causes, man induced causes (overexploitation of aquifers) or others (sea level rise, global change) seawater is invading aquifers in large parts of the world. Good management of the precious fresh water resources is crucial since coastal areas are the most densely populated regions of the world. About 50% of the world’s population lives in these coastal areas, a figure which will probably rise to 75% during the first century of the second millennium (Finkl, 1994). Tools need to be developed to help with this management. This dissertation aims to be a small contribution to that, more specifically in the realm of solute transport.

1.2 Focus on solute transport

Solute transport is of concern in many hydrogeological problems. Historically, first interest in solute transport in aquifers arose because of the problem of seawater intrusion. This was and still is a very practical and acute problem in coastal areas where one needs to keep production wells fresh. It was soon realised that solute transport must be considered as advective and dispersive transport. The way we are dealing with dispersive transport is still an ongoing area of research. A second major field of research was the spreading and fate of radionuclides in groundwater. This pointed to the importance of chemical reactions in groundwater. The water quality that is observed, is determined by different interacting chemical reactions along a flowpath. In the 1970s transport of anthropogenic contaminants originating from waste disposal sites and spills joined the research.

Today, solute transport is important as never before due to increasingly stringent remediation and environmental protection standards. It is now realised that groundwater is not an inexhaustible natural resource. Groundwater is very vulnerable to contamination as a result of agricultural, industrial and urban activities. Society has to deal with both historical and ongoing unavoidable contamination of the environment. This means that the characterisation, evaluation and remediation of aquifers with respect to groundwater contamination and solute transport will remain topical. It must be realised that this needs a multidisciplinary approach since physical, chemical and (micro)biological processes interact continuously in aquifers.

Problems with solutes in groundwater are often, not to say mostly, very practical ones and are requiring quantitative answers: when will a contaminant reach a production well, at what concentration, how long will remediation of a site take to clean it to a certain threshold level, etc… Therefore, hydro(geo)logists want to perform calculations, not only because it is fun but also because it is a necessity. Whereas before the introduction of powerful desktop computers simple calculations were performed with analytical derived formulas, numerical modelling is now widely used. Many fine computers programs have thus been developed through the years that brought numerical simulations available to the practitioner in the field. Modelling must be seen as an essential step in dealing with many solute transport problems and more generally in many hydrogeological issues. As already pointed out, a groundwater reservoir is complex with several physical, chemical and (micro)biological processes interacting. Besides helping in the answering of quantitative questions, models also provide insight in the system under study. Zheng & Bennet (2002) state that the most important use of simulation is not directly the predictive calculation but the investigation process itself. Indeed, by ‘playing’ with the model, characteristics of the system can be recognised which are invaluable when one ultimately dares to do some quantitative prediction. This ‘playing’ is all the more interesting when it is done following certain procedures. For instance, most parameters used in the model are subjected to uncertainties. Consequences of these uncertainties can be addressed through modelling. Certain parameters can also be correlated. Hill (1998) provides a practical set of modelling guidelines in a framework of sensitivity analyses and inverse modelling.

So, many arguments can be quoted in favour of modelling in hydro(geo)logical practice. After all, a model is the ultimate integration of all knowledge (hydrological data, lithological data,
Chapter 1: Introduction

A. Vandenbohede

sedimentological data, water quality, geophysical data, etc) available about a certain problem. When observations can be analysed and explained, it can be assumed that at least some basic insight in the problem under investigation is gained. This is far more valuable than only explaining observations in qualitative and descriptive terms. However, these benefits are also its weaknesses: the model is as good as the information one put into it! This leads to two major questions in hydrogeological modelling practice.

![Figure 1.3](image)

**Figure 1.3 Possible sources of contamination of aquifers.**

The first problem deals with the used parameters. In a steady state model, hydraulic conductivity of all layers and the hydraulic resistance between layers must be known. Specific elastic storage of every layer and storage coefficient near the water table is obligatory input for unsteady state flow. Dealing with solute transport, porosity and dispersivities are additional input parameters. Further, there is the infiltration rate and boundary conditions. Therefore, tests must be developed to derive hydraulic and solute transport parameters. It is thereby our view that such tests must be performed under controllable field circumstances. Pumping tests and tracer tests are very interesting tools for this purpose and are classically very often used. Hydraulic aquifer properties are studied with pumping tests and tracer tests aim to derive solute transport characteristics. This can be taken a step further in a test combining these two and analysing drawdown (or head) and concentration observations together. The first part of this dissertation focuses on the development of the combination of a pumping and tracer test into a forced gradient tracer test. This innovative combination of these two tests and the observations of concentration with geophysical borehole logging techniques lead to reliable parameter identification. Although the main focus of this dissertation is on physical processes a test to study chemical reactions in situ is also discussed, namely a push-pull test.

The second problem deals with implementation of the parameters into larger, regional models of groundwater flow. This problem is indissoluble connected to the problem of aquifer heterogeneity. Aquifers are heterogeneous media. We can have a basic idea about aquifer heterogeneity by drillings and all kind of measurements performed in the borehole or perhaps, if available, on cores. But
drillings are costly, so only a limited number of them are available. This means that only limited knowledge about the aquifer heterogeneity is available, depending on the number of drillings and other information. Parameters derived in the field are influenced by the geology of the field site. Performing the same test in the same lithological unit but on another site can therefore result in slightly different parameters, depending on the degree of aquifer heterogeneity. In practice, if one is lucky all but a few site are available where hydraulic and or solute transport parameters are determined in the model region. Dealing with this problem is the more important when solute transport is to be modelled because the seepage velocity is function of hydraulic conductivity and porosity. Dispersivity is directly a consequence of heterogeneity in aquifers, resulting in different values observed on different scales. So, heterogeneity has an important effect on groundwater flow in general and solute transport in particular but this heterogeneity is not completely known. Therefore, some general guidelines are needed based on the one dealing with modelling in general (Hill, 1998) but for solute transport in particular. The second part of this dissertation discusses and illustrates how the parameters derived on field sites can be implemented in practical hydrogeological problems and in larger scale (regional) models. Results of a parameter identification test and a push-pull test are directly used in the design of a remediation strategy for a contaminated site. Further with two field cases in the Belgian coastal plain, it is shown how modelling provides basic insights into the groundwater flow, solute transport and interaction of different parameters on them integrating available geological and hydro(geo)logical data.

1.3 Structure of the dissertation

This dissertation is structured as follows. In chapter 2, basic descriptions about governing equations in groundwater and solute transport are given with an overview of the parameters determining these equations and the methods to derive these parameters. The origin and influence of heterogeneity on hydraulic and solute transport parameters is discussed in chapter 3, especially the consequences on hydraulic conductivity and dispersivity. Chapter 4 treats the analyses of pumping tests and tracer tests. The combination in one test, the forced gradient tracer test and method of obtaining concentration observation are discussed. The novel interpretation of both drawdown and concentration observations with a numerical model is presented. The question if tracer tests and pumping tests derive compatible parameter values is discussed. A test to study chemical and (micro)biological processes is also given. Chapter 5 shows three applications were forced gradient tracer tests and push pull tests (for chemical and (micro)biological parameters) have been performed. The effect of aquifer heterogeneity on pumping test interpretation is explored in chapter 6. Chapter 7 deals with the applicability of the derived parameters. Different scales are identified. Direct application on the same scale as which the parameters are derived can be found in different in situ remediation schemes of contaminated sites. For regional scale applicability, some modelling and calibration guidelines are presented and illustrated with two groundwater flow models situated in the Belgian coastal plain. Finally, chapter 8 draws conclusions of this dissertation.
Chapter 2

On Groundwater Flow, Solute Transport and Parameter Identification Tests

The chess-board is the world; the pieces are the phenomena of the universe; the rules of the game are what we call the laws of nature. (Thomas H. Huxley)

2.1 Groundwater flow

2.1.1 Darcy's law

Darcy studied on experimental basis the flow of water through sand. Results were published in 1856. Figure 2.1 shows his experimental set up. A cylinder with cross-sectional area A (m²) is filled with sand and water flows through it. Two manometers are set on the inlet and on the outlet. These are small open tubes in which water can rise. The level to which the water rises, is function of the energy the water has (or pressure) at the inlet of the tube. The two manometers are a distance Δl (m) apart and h₁ and h₂ are respectively the level to which water rises (m) at the inlet and outlet of the cylinder.

![Figure 2.1 Experimental set-up used by Darcy.](image)

Q (m³/d) is the volume of water flowing through the cylinder per unit of time, Q/A (or q) is the volumetric flow rate per unit of surface area and (h₁-h₂)/Δl is the hydraulic gradient i over the cylinder. Darcy’s law expresses as:

\[
\frac{Q}{A} = -K \frac{(h₁ - h₂)}{Δl} = -Ki
\]

The velocity of flow is thus proportional to the hydraulic gradient. The negative sign indicates that the direction of flow is in the direction of decreasing water level. K (m/d) is a constant of proportionality. It is called the hydraulic conductivity and has unit of velocity.
Some points in Darcy’s law need further clarification. Water only flows through pores. So, a volumetric flow rate per unit area of connected pore space \( v \) (m/d) must be defined:

\[
\frac{Q}{n_e A} = \frac{q}{n_e} = v
\]  

where \( n_e \) is the effective porosity, the percentage of interconnected pore space. Then \( q \) is called the Darcy-velocity and \( v \) is called the seepage velocity (or linear or pore velocity) of groundwater flow. The seepage velocity is, however, also not the true velocity with which particles move in the porous medium. Due to tortuous movements around the sand particles, fluid particles travel a larger distance than \( \Delta l \). The actual particle velocity thus exceeds \( \Delta l / \Delta t \). The seepage velocity, however, gives the apparent velocity in terms of linear distance along the general flow directions in field or laboratory problems. This is a quantity that can be measured or calculated.

What is the meaning of water level measurements? A piezometer is the equivalent of the manometer in Darcy’s test. It is a well with open ends. Water is allowed to flow in the well freely. Bernoulli’s equation can then be applied. Under conditions of steady flow, the total energy of incompressible fluids is constant at all position along a flow path in a closed system:

\[
g z + \frac{P}{\rho_w} + \frac{v^2}{2g} = \text{constant}
\]  

\( g \) (m/d²) is the acceleration of gravity, \( z \) (m) is the elevation of the base of the piezometer, \( P \) (Pa) is the pressure exerted by the water column, \( \rho_w \) (kg/m³) is the fluid density and \( v \) (m/d) is the seepage velocity. The equation can be rewritten as:

\[
z + \frac{P}{\rho_w g} + \frac{v^2}{2g} = \text{constant}
\]  

The first term is the energy due to the position of the piezometer inlet. It is called the elevation head and equals the elevation of the base of the piezometer. The second term is the energy due to the sustained fluid pressure. It is called the pressure head and is the height of the water column in the piezometer. The third term is due to the fluid movement and is called the velocity head. Groundwater flow velocities are, however, that slow that this term can be ignored. Total hydraulic head is therefore:

\[
h = z + \frac{P}{\rho_w g}
\]  

In a field situation, hydraulic gradient vary in \( x \), \( y \) and \( z \) direction. Therefore, Darcy’s law is expressed as:

\[
q_x = -K_x \frac{\partial h}{\partial x} \quad q_y = -K_y \frac{\partial h}{\partial y} \quad q_z = -K_z \frac{\partial h}{\partial z}
\]  

The hydraulic gradient gives thus rise to a scalar field where the gradient of this field is:

\[
\nabla h = \nabla h = i \frac{\partial h}{\partial x} + j \frac{\partial h}{\partial y} + k \frac{\partial h}{\partial z}
\]  

where \( i \), \( j \) and \( k \) are unit vectors in the \( x \), \( y \) and \( z \) direction. In vectoral notation if hydraulic conductivity in \( x \), \( y \) and \( z \) direction are equal, Darcy’s law is:
The gradient of \( h \) is a vector that represents the spatial rate of change of hydraulic head and consists of three components \( x, y \) and \( z \), each of which represents how fast the head changes in that respective direction.

In the general case, the hydraulic conductivity tensor has nine components. However, the coordinate axes can normally be assumed to coincide with the principal components of the hydraulic conductivity tensor \( (K_{xx}, K_{yy}, K_{zz}) \) or simply \( (K_x, K_y, K_z) \), which are generally normal or parallel to stratum bedding. In this case, the cross terms \( (K_{xy}, K_{xz}, K_{yx}, K_{yz}, K_{zx}, K_{zy}) \) become zero. This assumption is incorporated in most commonly used flow models.

A final consideration by Darcy’s law concerns the hydraulic conductivity. It is the amount of water that flows through a unit cross-sectional area per unit of time and under unit of hydraulic gradient. Conductivity is a function of the characteristics of the porous medium and of the fluid. The parameter characterising only the conductive properties of the medium is called the intrinsic permeability. The relation between the hydraulic conductivity, \( K \), and the intrinsic permeability, \( k \) (m\(^2\)), is:

\[
K = k \frac{\rho_w g}{\mu}
\]

where \( \mu \) (kg/md) is the dynamic viscosity of the water.

### 2.1.2 Groundwater flow equation

The mathematical treatment of the groundwater flow equation through a porous medium depends upon an equation that captures the essence of the physics of flow. The basis for developing such an equation is a conservation statement that balances the inflow, outflow and change in water mass within a representative volume of porous medium. A conservation of fluid mass statement may be given as:

mass inflow rate − mass outflow rate = change in mass storage with time

---

**Figure 2.2** Representative volume of porous material.
Consider a unit volume filled with water saturated porous medium with unit length $\Delta x$, $\Delta y$ en $\Delta z$ (figure 2.2). Mass inflow rate through side ABCD is

$$\rho_w q_x \Delta y \Delta z$$  \hspace{1cm} 2.10

with $\rho_w$ the water density (kg/m$^3$) and $q_x$ the Darcy velocity in the x-direction (m/d). Mass outflow through the side EFGH is

$$\left( \rho_w q_x + \frac{\partial (\rho_w q_x)}{\partial x} \right) \Delta y \Delta z$$  \hspace{1cm} 2.11

Mass inflow and outflow respectively through the sides CDHG and BAEF are:

$$\rho_w q_y \Delta x \Delta z$$  \hspace{1cm} 2.12

$$\left( \rho_w q_y + \frac{\partial (\rho_w q_y)}{\partial y} \right) \Delta x \Delta z$$  \hspace{1cm} 2.13

with $q_y$ the Darcy velocity in the y-direction (m/d).

Mass inflow and outflow respectively through the sides ADHE and BCGF is:

$$\rho_w q_z \Delta x \Delta y$$  \hspace{1cm} 2.14

$$\left( \rho_w q_z + \frac{\partial (\rho_w q_z)}{\partial z} \right) \Delta x \Delta y$$  \hspace{1cm} 2.15

with $q_z$ the Darcy velocity in the z-direction (m/d).

Adding these results gives the net outflow rate (inflow minus outflow rate) through all the faces:

$$- \left( \frac{\partial (\rho_w q_x)}{\partial x} + \frac{\partial (\rho_w q_y)}{\partial y} + \frac{\partial (\rho_w q_z)}{\partial z} \right) \Delta x \Delta y \Delta z$$  \hspace{1cm} 2.16

Net outflow rate per unit volume is:

$$- \left( \frac{\partial (\rho_w q_x)}{\partial x} + \frac{\partial (\rho_w q_y)}{\partial y} + \frac{\partial (\rho_w q_z)}{\partial z} \right) = -\nabla . (\rho_w q) = -div(\rho_w q)$$  \hspace{1cm} 2.17

The divergence of $\rho_w q$ describes change in mass flux per unit volume. The net mass outflow is due to changes in the storage capacity of the unit volume, $\rho_w n_e$ is the liquid mass per unit volume. One gets:

$$div(\rho_w q) = \frac{\partial (\rho_w n_e)}{\partial t}$$  \hspace{1cm} 2.18

If water density is equal in all directions:
\[-\left(\frac{\partial (q_x)}{\partial x} + \frac{\partial (q_y)}{\partial y} + \frac{\partial (q_z)}{\partial z}\right) = \frac{1}{\rho_w} \frac{\partial (\rho_w n_e)}{\partial t}\]  

2.19

Substitution of Darcy’s law gives:

\[
\frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) = \frac{1}{\rho_w} \frac{\partial (\rho_w n_e)}{\partial t}\]  

2.20

The expression has a positive sign because of the negative sign in Darcy’s law. Assuming the material is isotropic and homogenous, the left hand site of this last equation becomes:

\[
K \left( \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} \right)\]  

2.21

The term \(\partial^2 h/\partial x\partial y\) represents a space change in the gradient across the unit volume. Accordingly, there must follow velocity variations in the three component directions. If increases in \(x\) are compensated by decreases in \(y\) and so forth, the fluid mass per unit volume is not changing with time. Then:

\[
 \left( \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} \right) = 0\]  

2.22

This is Laplace’s equation. The solution to this equation describes the value of the hydraulic head at any point in a three-dimensional flow field.

Another possibility is the case where the unit volume has some storage qualities. It is assumed that the gains or losses in fluid volume within the unit volume are proportional to changes in hydraulic head. An increase in head suggests that water has gone into storage and a decrease in head suggests the opposite, the removal of water from storage. To account for these gains and losses, the right hand site of the groundwater flow equation becomes:

\[
\frac{1}{\rho_w} \frac{\partial (\rho_w n_e)}{\partial t} = S_s \frac{\partial h}{\partial t}\]  

2.23

where \(S_s\) is the specific elastic storage (m\(^{-1}\)). It is the volume of water withdrawn from or added to the unit volume when the head changes a unit amount. The specific elastic storage is due to compressibility of the water and of the porous medium and can be expressed as:

\[
S_s = \rho_w g \left( \beta_p + n \beta_w \right)\]  

2.24

where \(\beta_p\) is the vertical compressibility of the porous medium and \(\beta_w\) is the fluid compressibility both with units of pressure\(^{-1}\).

Rearrangement of equation 2.20 than gives:

\[
\left( \frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} \right) = \frac{S_s \frac{\partial h}{\partial t}}{K}\]  

2.25
which is called the diffusion equation. The quantity $K/S_s$ is called the hydraulic diffusivity and has the unit m²/d. It describes, in contrast with Laplace’s equation, the unsteady or transient flow. The solution to this equation describes the value of the hydraulic head at any point in a three-dimensional-flow field at any given time or, more precisely, how the head is changing with time at any place.

So, groundwater flow is governed by Laplace’s equation in the case of steady state flow and by the diffusivity equation in the case of unsteady state flow. They can be expressed very concisely as:

$$\nabla^2 h = 0$$

$$\nabla^2 h = \frac{S_s}{K} \frac{\partial h}{\partial t}$$

### 2.2 Solute transport

Mass that is dissolved in groundwater undergoes transport and redistribution with flow. The main transport processes of concern in groundwater include advection, dispersion, adsorption, biodegradation and chemical reactions (Domenico & Schwartz, 1997). Advection is a mass transport process due to the flow of water in which mass is dissolved. The direction and rate of transport coincides with the groundwater flow. This process determines therefore when a mass dissolved in groundwater is observed at a certain place. Advection is completely determined by seepage velocity. Seepage velocity $v$ (m/d) is function of hydraulic conductivity $K$(m/d), effective porosity $n_e$ (-) and the hydraulic gradient $\partial h/\partial l$ (-).

$$v = -\frac{K}{n_e} \frac{\partial h}{\partial l}$$

Knowledge of groundwater flow is directly transferable to understanding advection i.e. head differences over columns in laboratory experiments, drawdowns around pumping wells, regional head distributions in regional problems, etc. are to be studied along with the geological layering. Mass added to a stream tube will remain in it if only advection is taking place. Dispersion mixes mass between stream tubes. Because advection is the mean transport in groundwater, it should be first dealt with in treating solute transport before looking at more complex phenomena.

Mass may alter groundwater flow. This is the case when density effects come into play. High concentrations of salt alter the density of water and thus alter the groundwater flow and advection considerably. Modelling such flow should account for these density effects and a density term must be added.

Dispersion (or hydrodynamic dispersion) is a process of fluid mixing that causes the development of a mixing zone between the dissolved mass and the displaced fluid with different composition. This can be illustrated with the classic column experiments. Fresh water in a column filled with porous material is displaced by salt water leaking on top of it. As the front of salt water evolves in the column, the transition zone between the two water qualities will grow. Even so if a plume of salt water is injected in fresh water, the centre of this plume will move according to advection but a transition zone will develop between the fresh and salt water. This transition zone will enlarge with time. Dispersion determines therefore which concentrations are observed at a certain place and time. This process is traditionally described by the solute transport parameters, longitudinal and transverse dispersivity. Dispersion occurs in porous media because of two processes, diffusion and mixing due to velocity variations. This later process is called mechanical dispersion.
Adsorption is the partitioning of organic contaminants from the soluble phase into the soil matrix. The result is the developments of retardation fronts. Biodegradation represents the transformation of certain organics to simple carbon dioxide and water (or intermediate products) in the presence of microbes, bacteria, etc. in the subsurface. Chemical processes (acid-base reactions, solution, exsolution, volatilisation, precipitation, complexation reactions, reactions on surfaces, oxidation-reduction reactions, hydrolysis, isotopic processes, etc) may complicate solute transport further.

### 2.3 Diffusion and mechanical dispersion

#### 2.3.1 Diffusion

Chemical mass flux $J$ (moles/cm²s) is proportional to the concentration gradient. This is expressed for a simple aqueous nonporous medium by the Fick’s law:

$$ J = -D_d \text{grad}(C) $$

where $C$ is the concentration (moles/cm³) and $D_d$ (cm²/s) a proportionality constant, termed the diffusion coefficient. Random molecular motion due to thermal kinetic energy causes molecular diffusion. The coefficient describing this scattering is larger in gases than in liquids and larger in liquids then in solids due to molecular spacing. Diffusion coefficient in porous media is smaller than in pure liquids primarily because collision with the solids of the medium hinders diffusion. Introduction of a bulk diffusion coefficient $D'_{d}$ to account for effects of tortuosity gives the statement most commonly referred to as Fick’s law for diffusion in sediments:

$$ J = -D'_{d} n \text{grad}(C) $$

Where $n$ is the porosity. In the absence of an evaluation for $D'_{d}$, an effective diffusion coefficient $D_d= D'_{d} n$ is generally employed so that:
Several different empirical approaches are composed defining an effective diffusion coefficient in function of porosity and or tortuosity.

\[ J = -D \ast \text{grad}(C) \]  

Figure 2.4. Various processes involving solute transport in porous media (Oude Essen, 2000).
2.3.2 Mechanical dispersion

Mechanical dispersion is mixing caused by velocity variations around a mean flow velocity. It is therefore an advective process and not a chemical one. These variations are caused by nonidealities (heterogeneities) in the porous medium. Both effective porosity and hydraulic conductivity heterogeneity of the porous medium result in these velocity variations. Hydraulic conductivity is considered as the major factor herein because of its lognormal distribution in the groundwater reservoir.

Heterogeneities are encountered on different scales. Every scale has typical nonidealities (Alpay, 1972):

- **Microscopic heterogeneity: pore to pore**
  1. Pore size distribution
  2. Pore geometry
  3. Dead-end space
- **Macroscopic heterogeneity: well to well or intraformational**
  1. Stratification characteristics
     - Nonuniform stratification
     - Stratification contrasts
     - Stratification continuity
     - Insulation to cross-flow
  2. Permeability characteristics
     - Nonuniform permeability
     - Permeability trends
     - Directional permeability
- **Megascopic heterogeneity: formational (either fieldwide or regional)**
  1. Reservoir geometry
     - Overall structural framework: faults, dipping strata, etc.
     - Overall stratigraphic framework: bar, blanket, channel, etc.
  2. Hyperpermeability-oriented natural fracture systems

Nonidealities on all of these scales are responsible for mechanical dispersion. Variability in velocity on microscopic scale for example develops because of differing flow regimes across individual pore throats and/or variability in the tortuosity of the flow channels. Contrast of hydraulic conductivity among and sedimentation structures within layers cause for instance velocity variations on a macroscopic scale.

2.4 Dispersion coefficient on microscopic scale

The coefficient of hydrodynamic dispersion is the sum of the coefficients of bulk diffusion ($D^*_{d}$) and mechanical dispersion ($D'$). Values of the bulk diffusion coefficient can be estimated reasonably well within an order of magnitude for granular media. Mechanical dispersion and its relative importance can be less accurately estimated.

Column experiments have shown some major relationships concerning the dispersion coefficient. Therefore Pfannkuch (1962) defined the dimensionless numbers $D_l/D_d$ and $v_d/m_D$, where $v$ is the seepage velocity, $m_D$ is the mean grain size, $D_l$ is the longitudinal dispersion coefficient and $D_d$ is the diffusion coefficient. $D_l/D_d$ normalises the observed dispersions in the column by dividing it by the coefficient of diffusion of the tracer in water. $v_d/m_D$ is the Peclet number, a ratio expressing advective to diffusive transport. Figure 2.5 shows relationships developed by Pfannkuch (1962) with four classes of mixing related to the Peclet number. Class 1 is for small values of the Peclet number (less then
0.01). $D_L/D_d$ does not change in relation to the Peclet number, which means that diffusion is the main cause of mixing. With increased values of the Peclet number, mixing is caused by both diffusion and mechanical mixing. In class 3, mechanical dispersion dominates the mixing process. Class 4 has Peclet numbers in the order of $10^4$-$10^6$. The effects of molecular diffusion are negligible. Also shown in figure 2.5 is the ratio $D_T/D_d$ where $D_T$ is the transverse dispersion coefficient (from Perkins and Johnston, 1963). Dispersion in two dimensions causes spreading in the longitudinal and transverse directions both ahead of and lateral to the advective front. The two curves in figure 2.5 are similar in shape, indicating that the process of transverse mixing is much the same as longitudinal mixing. Longitudinal dispersion is however larger than transverse dispersion at a given Peclet number. When Peclet number is for instance larger than 100, longitudinal dispersion is approximately 10 times larger than transverse dispersion. This tendency applies not only at microscopic but also on larger scales.

![Figure 2.5 D_L/D_d and D_T/D_d in function of Peclet number (Pfannkuch, 1962).](image)

One important result of the study of column tests is the determination that longitudinal dispersion is proportional to velocity. These relationships have been generalised to macroscopic and megascopic scales and are:

$$D_L = \alpha_L v$$ and $$D_T = \alpha_T v$$

2.31

Dispersion coefficients are expressed as m²/d and seepage velocities as m/d. $\alpha_L$ and $\alpha_T$ are the longitudinal and transverse dispersivity of the medium (m). Dispersivity is considered a characteristic property of a porous medium. In practice they quantify mechanical dispersion in a system. There are actually two transverse dispersivities measured at 90° to each other. For example, with horizontal flow, one component of transverse spreading will occur in the horizontal plane, and the second will occur in the vertical plane.

In most modelling studies, use of a coefficient of hydrodynamic dispersion implies that the behaviour is Fickian. This means that the transport of a quantity in a direction of a concentration gradient at a rate that is proportional to the gradient. While this relationship describes molecular diffusion, it is not a mechanistically correct representation of mechanical dispersion. The justification of the diffusional model used for mechanical dispersion is a practical one. The net effect of dispersion is the development of normal or Gaussian concentration distribution. It is argued that although the microscopic mechanism for diffusion and mechanical dispersion differ completely, the macroscopic outcome for both processes is quite similar: a normal concentration distribution.

Xu & Eckstein (1997) have made statistical analysis of the relationships between dispersivity and different physical properties of the porous medium in column tests. They conclude that porosity and the uniformity of grain size are the two most important factors affecting dispersivity. Dispersivity increases as uniformity decreases which means that dispersivity is proportional with the degree of
heterogeneity. Dispersivity increases with decreasing porosity. If the material is uniform (homogeneous), dispersivity is proportional to median grain size. No evidence is found of a relation between dispersivity and hydraulic conductivity. The effect of local variations in hydraulic conductivity was hereby not considered.

2.5 Derivation of the Advection-Dispersion Equation (ADE) for solute transport

2.5.1 Derivation of the ADE

Derivation of the advection-dispersion equation (ADE) is based on the law of conservation of mass. The derivation is based on those of Ogata (1970) and Bear (1972) and is presented in Freeze and Cherry (1979). It is assumed that the porous medium is homogeneous, isotropic and saturated. The flow is steady state and Darcy’s law applies. The flow is described by the average linear velocity or seepage velocity, which transports the dissolved mass by advection. Hydrodynamic dispersion is used to account for the additional spreading caused by fluctuations in the velocity field.

Consider the solute flux in and out of an elemental volume. In Cartesian coordinates, the specific discharge or Darcy velocity $q$, has components $q_x$, $q_y$ and $q_z$ and the average seepage velocity $v = q/n_e$ has the components $v_x$, $v_y$ and $v_z$. The rate of advective transport is equal to $v$. The concentration of the solute $C$ is defined as the mass of solute per unit volume of solution. The mass of solute per unit volume of porous media is therefore $n_eC$. For a homogeneous medium with constant effective porosity $n$ it follows that

$$\frac{\partial (nC)}{\partial x} = n_e \left( \frac{\partial C}{\partial x} \right) \quad 2.32$$

The mass of solute transported in the x direction by the two mechanisms of solute transport can be represented as:

Transport by advection is $v_x n_e C dA$

$$2.33$$

Transport by dispersion is $n_e D_x \frac{\partial C}{\partial x} dA$

where $D_x$ is the hydrodynamic dispersion coefficient in the x direction and $dA$ is the elemental cross-sectional area of the cubic element. The dispersion coefficient $D_x$ is related to the dispersivity $\alpha_x$ and the diffusion coefficient $D_d$ by

$$D_x = \alpha_x v + D_d \quad 2.34$$

The form of the dispersive component is analogous to Fick’s first law.

If $F_x$ represents the total mass of solute per unit cross-sectional area transported in the x direction per unit time, then

$$F_x = v_x n_e C - n_e D_x \frac{\partial C}{\partial x} \quad 2.35$$
The negative sign before the dispersive term indicates that the contaminant moves towards the area of lower concentration. Similar expression can be derived for the x and z directions:

\[
F_y = v_y n_e C - n_e D_y \frac{\partial C}{\partial y} \tag{2.36}
\]

\[
F_z = v_z n_e C - n_e D_z \frac{\partial C}{\partial z} \tag{2.37}
\]

The total amount of solute entering the fluid element is

\[
F_y dzdy + F_y dzdx + F_z dxdy \tag{2.38}
\]

The total amount leaving the representative fluid element is

\[
\left( F_x + \frac{\partial F_x}{\partial x} dx \right) dydz + \left( F_y + \frac{\partial F_y}{\partial y} dy \right) dx dz + \left( F_z + \frac{\partial F_z}{\partial z} dz \right) dx dy \tag{2.39}
\]

The difference in the amount entering and leaving the fluid element is

\[
\left( \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right) dx dy dz \tag{2.40}
\]

Because the dissolved tracer is assumed to be conservative (nonreactive), the difference between the flux into the element equals the amount of dissolved substance accumulated in the element. The rate of mass change in the element can be represented by

\[
- n_e \frac{\partial C}{\partial t} dx dy dz \tag{2.41}
\]

The complete conservation of mass expression, therefore, becomes

\[
\left( \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right) = - n_e \frac{\partial C}{\partial t} \tag{2.42}
\]

Substitution of expressions for \( F_x, F_y \) and \( F_z \) and cancellation of \( n \) from both sides of the equation yields:

\[
\left( \frac{\partial}{\partial x} \left( D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial C}{\partial z} \right) \right) - \left( \frac{\partial}{\partial x} (v_x C) + \frac{\partial}{\partial y} (v_y C) + \frac{\partial}{\partial z} (v_z C) \right) = \frac{\partial C}{\partial t} \tag{2.43}
\]

In a homogeneous medium in which the velocity is steady and uniform (that is, it does not vary through time or space) and the dispersion coefficients \( D_x, D_y \) and \( D_z \) do not vary through space (but \( D_x \neq D_y \neq D_z \)), the equation becomes:

\[
\left( D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \right) - \left( v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} \right) = \frac{\partial C}{\partial t} \tag{2.44}
\]
This three-dimensional solute transport equation is difficult to solve in field cases of practical interest due to aquifer characteristics and boundary conditions. Numerical approaches are normally used therefore. There are, however, a few limited number of relatively simple, one-dimensional problems for which analytical solutions exist. Full treatment of this can be found in literature, Domenico & Schwartz (1998) provide an excellent starting point. Two-dimensional and fully three-dimensional modelling is in many cases appropriate. Analytical models have been developed for certain simplified initial and boundary conditions. Numerous analytical models are available in literature (Bear, 1979; Hunt, 1978; Wilson and Miller, 1978; Cleary and Ungs, 1978; Shen, 1976, Galya, 1987; Javandel et al., 1984) for pulse and continuous contaminant sources, with boundary conditions ranging from no flow to constant head. Processes as advection, dispersion, adsorption and first order decay (biological or radioactive) can be included.

2.5.2 Hydrodynamic dispersion

The diffusion term in hydrodynamic dispersion is under normal flow conditions of marginal importance with respect to the mechanical dispersion term. The subdivision of hydrodynamic dispersion into mechanical dispersion and molecular diffusion is artificial. The dispersion coefficient, which is a second-rank symmetrical tensor, is given by Scheidegger (1961):

\[
D_{ij} = \frac{\alpha_{ijmn} v_m v_n}{|v|} \\
D_{ii} = \alpha_T |v| \delta_{ij} + \frac{(\alpha_L - \alpha_T) v_i v_j}{|v|}
\]

where \(D_{ij}\) is the coefficient of mechanical dispersion (m²/d), \(\alpha_{ijmn}\) is the geometrical dispersivity tensor of the aquifer (m), \(v_m\) and \(v_n\) are the components of the seepage velocity in \(m\) and \(n\) direction (m/d), \(|v|\) is the magnitude of the seepage velocity (m/d) and \(\delta_{ij} = 1\) if \(i=j\) or \(\delta_{ij} = 0\) if \(i\neq j\). Scheidegger defines the dispersivity tensor for an isotropic aquifer in terms of two constants:

\[
D_L = \alpha_L |v| \quad \text{and} \quad D_T = \alpha_T |v|
\]

The components for hydrodynamic dispersion for three-dimensional flow in an isotropic aquifer, considering mechanical dispersion as well as molecular diffusion \(D_m\) are as follows:

\[
D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D_m \\
D_{yy} = \alpha_T \frac{v_x^2}{|v|} + \alpha_L \frac{v_y^2}{|v|} + \alpha_T \frac{v_z^2}{|v|} + D_m \\
D_{zz} = \alpha_T \frac{v_x^2}{|v|} + \alpha_T \frac{v_y^2}{|v|} + \alpha_L \frac{v_z^2}{|v|} + D_m \\
D_{xy} = D_{yx} = \frac{(\alpha_L - \alpha_T) v_x v_y}{|v|}
\]
2.6 Parameter identification

2.6.1 Introduction

For modelling of solute transport, one needs to know certain parameter values. Parameters are divided for practical purpose in hydraulic and solute transport parameters. Horizontal and vertical (hydraulic) conductivity and specific elastic storage are the hydraulic parameters, longitudinal and transverse dispersivity and effective porosity are the solute transport parameters. Over the years, different tests have been designed to produce one or more parameters. The next two entries aim to give an overview of the most common hydraulic and solute transport parameter tests available.

2.6.2 Hydraulic parameter identification tests

Permeameter tests are laboratory tests to derive the hydraulic conductivity of a soil sample that is assumed to be undisturbed. A hydraulic gradient is imposed on the sample and water is allowed to flow through it. In a constant head permeameter, this gradient is kept constant and the volume of water flowing through the sample is measured in function of time. In a falling head permeameter, the head at the inlet of the cylinder containing the sample is allowed to fall. Falling of this head in function of time is measured. Interpretation of measurements is done with Darcy’s law in both cases. Extrapolations of results to field scale and aquifer conductivity are questionable due to the scale of the test.

Compressibility (and hence specific elastic storage) and hydraulic conductivity can be derived on laboratory scale with a consolidation test. A saturated soil sample is placed in a cell that is stressed. Different phases of loading and unloading can be accomplished. Same remarks as with the permeameter test must made. Extrapolations of results to field scale are questionable due to the scale of the test.

Permeameter and consolidation tests are direct tests. A number of indirect measurements of hydraulic conductivity are known in literature. Lebbe (1999a) for instance provides an overview. Relations between hydraulic conductivity and grain size distributions, gamma ray logs or electrical resistivity are available.

Well tests exist. They are all field tests and are performed in one well. Best know are the bail and slug tests. Thereby a volume (water or just a massive cylinder) is quickly extracted or added from or in the test well. The evolution of the water level to its equilibrium state is followed. The interpretation method of Bouwer and Rice (Bouwer, 1989) and Hvorslev (1951) are mostly used. Some remarks must be made with regards to the validity of the results. In these tests, only a small volume of aquifer is tested. Drilling disturbances of this test volume can be quit large and important. Derived hydraulic conductivity is thereby sum of the layer one wishes to test plus a zone affected by the drilling and the zone were calibrated sand screen are located. Both interpretation methods are based on the model of Thiem (1906) which is only a crude approximation of real field flow conditions.
The pumped layer is bounded above and below by an impervious layer and forming a confined layer with a seemingly infinite lateral extent. The pervious layer is homogeneous and has a constant thickness. The discharge rate is constant and the pumped well has a screen over the entire thickness of the layer. The flow approaches the steady state and the hydraulic head is almost constant during the last part of the test.

During a **pumping test**, one well (the pumping well) is pumped and the drawdowns in other wells (observation wells) are followed. Large volumes of the groundwater reservoir are thereby tested in situ and derived parameters are therefore more reliable for use in field problems. Different interpretations and models have been developed. The resulting groundwater flow towards the pumping well is treated by the radial groundwater flow equation:

\[
\frac{K_h}{r} \left( \frac{\partial^2 S}{\partial r^2} + \frac{1}{r} \frac{\partial S}{\partial r} \right) + K_v \frac{\partial^2 S}{\partial z^2} = \frac{S}{\partial t}
\]

\[2.48\]

\(K_h\) is the horizontal hydraulic conductivity, \(K_v\) the vertical hydraulic conductivity, \(S\) the specific storage, \(s\) drawdowns and \(r\) the distance from a pumping well and \(z\) the depth. With drawdowns observed during the execution of a pumping test, hydraulic parameters of the permeable layer can be calculated. Therefore, some analytical solutions are available in literature. Lebbe (1999a) gives an overview of the most used methods and their derivation from the groundwater flow equation. These derivations of analytical formula, however, require stringent boundary conditions. Here we want to discuss briefly the limitations of the most used analytical models (model of Theis, Jacob-Hantush, Hantush and Boulton-Cooley).

The model of Theis (1935) describes the unsteady state groundwater flow in a confined aquifer. For the solution of the groundwater flow equation, specific boundary conditions and assumptions are needed. The permeable layer is considered bounded above and beneath by an impermeable layer. Further, all layers are considered of infinite lateral extend, homogeneous and of constant thickness. Discharge rate is constant and the pumped well is screened over the entire thickness of the permeable layer. Diameter of the pumped well is very small so that well storage can be neglected. Considering these restrictions, horizontal hydraulic conductivity and specific storage of the permeable layer can be calculated from drawdown observations in a single well. Cooper and Jacob (1946) derived a slightly different interpretation technique based on the same assumptions as Theis. From these assumptions, the fact that permeable layer is bounded by impermeable layers is the most stringent. No such situation is encountered in nature and users of the model must be aware of the implications. Flow from the adjacent semi-permeable layers is totally neglected. Water that will leak in reality from these layers will result in smaller drawdowns than in the case of a confined aquifer. Interpreting these drawdowns with the model of Theis will lead to a derived hydraulic conductivity, which is too large. Using this conductivity to calculate travel times for solute transport for instance will lead to velocities that are too large. The amount of water leaking from the surrounding layers into the pumped layer can be quite large and so will be the reduction of the drawdown with respect to the Theis model drawdowns at the same distance. This effect is illustrated by the results of Wenzel (1942), the first to apply the model of Theis. Wenzel (1942) found the results depending strongly on the observation well (read distance from pumping well) he used. Using an observation well at large distance from the pumped well will lead to a larger hydraulic conductivity derived with the Theis method than using drawdowns from an observation well close to the pumped well. This apparent scale effect is of course due to the stringent boundary conditions rather than being a real physical property of the sediments. The farther from the pumping well one makes drawdown observations, the larger the error becomes by neglecting hydraulic leakage.

Applicability of the model of Theis is very limited and it was adjusted very soon. However, the model of Theis is until now one of the most used method in hydrogeology albeit wrongly in many cases. Unsteady state flow in a semi-confined aquifer was first treated by Jacob (1946) and further adjusted by Hantush and Jacob (1955). According to this model, Walton (1962) presented a new interpretation
method. With the model of Jacob-Hantush, horizontal hydraulic conductivity and specific elastic storage from a semi-confined aquifer can be derived from a time-drawdown curve, measured in an observation well at known distance from the pumping well. Hydraulic resistance of one of the bounding semi-permeable layers or the combined resistance of both semi-permeable layers can be calculated. In the model of Jacob-Hantush the permeable layer is bounded above and below by semi-permeable layers or by one impermeable layer and one semi-permeable layer. Other boundary conditions and assumptions are the same as for the Theis model. Leakage from the bounding semi-permeable layer(s) is however considered proportional to the drawdown in the permeable layer at every distance from the pumped well so that the storage decrease in the semi-permeable layer(s) is ignored. No drawdown is considered to occur at the upper and lower boundary of respectively the upper and lower semi-permeable layers. This means that the amount of pumped water coming from the semi-permeable layers is underestimated. Again this leads to a derived hydraulic conductivity of the permeable layer which is too large.

Storage decrease in the bounded semi-permeable layers is accounted for in the model of Hantush (1960). The model is an extension of the theory of the radial flow toward a pumped well with a complete screen in a semi-confined aquifer and with a constant discharge rate. To solve the partial differential flow equation, a constant hydraulic head is assumed at top of the superjacent layer and at the base of the subjacent layer. One of the surrounding layers can also be treated as impermeable. In reality however, this constant head boundaries will only be encountered if the surrounding layers are permeable enough. Although the model of Hantush features a more realistic solution of the flow equation, hydraulic conductivity of the permeable layer will be calculated too large.

The above mentioned models do not consider water table movements. Boulton (1955), Cooley (1971,1972) and Cooley en Case (1973) give a solution of the flow equation in the case where a water table is present in a semi-permeable layer above the pumped permeable layer. To solve the equation the specific elastic storage of the semi-permeable layer is, however, neglected.

These different analytical solutions of the partial differential groundwater flow equation have thus one common disadvantage: they tend to underestimate the flow from adjacent semi-permeable layers and therefore overestimate the horizontal conductivity of the pumped permeable layer. This overestimation increases with the observation distance of the used drawdowns. Analytical models are very rigid in boundary conditions and strict configurations of (semi-)permeable and impermeable layers are required. Although analytical models have struck root in literature and are ‘successfully’ used (which means they provide a solution) in pumping test interpretations, these drawbacks become dramatically apparent in tracer test interpretation. Velocities calculated with the hydraulic conductivities obtained by fitting inappropriate analytical models are often too high. This observation is often found in literature (see chapters 4 and 5). With the above mentioned analytical models, the user has also no indication of the accuracy with which the parameters are derived, only a solution is provided. Therefore, models that approximate more the real flow conditions have to be applied. Numerical models provide such a generalised interpretation method. With inverse numerical models hydraulic conductivity (horizontal and/or vertical) and specific elastic storage from permeable and semi-permeable layers can be derived together with their joint confidence region. So, not only the parameters can be deduced but one also has indications about their accuracy. The inverse numerical model for pumping test interpretation is fully treated in chapter 4.

Calibration of regional groundwater flow models can, in certain circumstances, be used to derive hydraulic parameters. These systems are however complex and initial and boundary conditions are not always known exactly. Discussion of regional groundwater flow models and the problem of parameterisation can be found in chapter 7.
2.6.3 Solute transport parameter identification tests

During a tracer test, a chemical component in the groundwater (the tracer) is followed. Aim is to deduce processes (advection, dispersion, chemical reactions, etc) of interest. Different tracers can be used:

- Natural occurring ions (Br-, Cl-, …)
- Environmental isotopes (²H, ³H, ¹⁸O, …)
- Contaminants
- Specific chemicals injected in the groundwater for the test, for instance radioisotopes (³H, ¹³¹I, ⁸¹Br), ions (Cl-, Br-) or organic components (rhodamine, fluoresceine, uranine).

This list can be divided in purposely injected tracers and tracer already occurring in the groundwater or also in reactive (non-conservative) and non-reactive (conservative) tracers.

Determination of the tracer used for a certain experiment depends on certain criteria. First of all, the type of process one wish to study is of importance. Study of behaviour and reactions of certain chemical components in the groundwater reservoir determines the type of tracer to be used. A second criterion is the scale of the test. In large scale tests (tens of kilometres), natural occurring tracers (natural occurring ions, environmental isotopes) are to be used. At smaller scales, contaminant plumes are often used. It is obviously not very responsible to inject large quantities of tracer from an environmental and ecological point of view. Small scale tracer tests use the injection of small amounts of tracer.

Different types of tests have been designed (Domenico & Schwartz, 1998). In a natural gradient test, a volume of tracer is injected in the groundwater reservoir and its evolution and spreading is monitored in time. The tracer moves only due to natural occurring gradients since no pumping is involved. Advection, dispersion and chemical reactions can be derived. If one ore more pumping tests or continues injection wells are used the test are generally called forced gradient tests. Many different lay-outs exist. In a single well pulse test, a volume of tracer is injected followed by water without the tracer. After the injection, the well is pumped with the same discharge rate of the injection phase and breakthrough of the tracer is observed. Longitudinal dispersivity and chemical reactions were classically studied with these kind of tests. Haggerty et al. (1998), however, show that dispersivity can not reliably be derived, so only chemical reactions can be followed with the single well pulse test. An injection and pumping well are used in the two well tracer test. Injection and pumping is performed at the same time. At the injection water a tracer is continuously added. The water pumped up can be reused for the injection. Observations can be made in the pumping well and advection, dispersion and chemical reactions can be studied. Wells in between injection and pumping well can be installed for more detailed observation. In a single well injection or withdrawal well with multiple observation wells, a transient radial flow field is installed. In a radially divergent test, the tracer movement away from an injection well is monitored. In a radially convergent test, the tracer is injected in one well and moves towards a pumping well. Observation wells are installed in between.

Gelhar et al. (1992) classify the welt of tracer tests in three reliability classes with respect to the derivation of dispersivity:

- High-reliability: dispersivity values are derived accurate within a factor of two
  - Ambient flow with known tracer input, diverging radial flow, two-well pulse test (without recirculation).
  - Tracer input is well defined
  - Tracer is conservative
  - Spatial dimensionality of the tracer concentration measurements is appropriate
  - Analysis of the tracer concentration data is appropriate
Low-reliability: dispersivity values are derived accurate within one or two orders of magnitude
- Two-well recirculating test with step input
- Single-well injection-withdrawal test with tracer monitoring at the single well
- Tracer input is not clearly defined
- Tracer breakthrough curve is assumed to be the superposition of breakthrough curves in separate layers
- Measurement of tracer concentration in space is inadequate
- Equation used to obtain dispersivity is not appropriate for the data collected

The third class is of intermediate reliability and falls somewhere between the extremes.
Chapter 3

Aquifer Heterogeneity
Effects on Hydraulic and Solute Transport Parameters

Felix qui potuit rerum cognoscere causas. (Virgilius)

3.1 Heterogeneity of groundwater reservoirs

Before looking at aquifer heterogeneity, some clear definitions should be made. Distinction must be made between heterogeneity and anisotropy. A volume of aquifer material is heterogeneous for a certain parameter if the value of this parameter depends on its position in space. In the other case, the volume of aquifer material is homogeneous. A volume of aquifer material is isotropic at a point for a parameter if this parameter value is independent of the direction of measurement at that point. A volume of aquifer material is anisotropic for a parameter at a point if the parameter value changes with the direction of measurement. An example of anisotropy is for instance the situation were the horizontal hydraulic conductivity is different from the vertical hydraulic conductivity. A volume of aquifer material can thus be homogeneous and isotropic, homogeneous and anisotropic, heterogeneous and isotropic or heterogeneous and anisotropic.

Groundwater reservoirs are, however, inherent heterogeneous and anisotropic. This is due to the depositional (or more general, the formational) history of natural materials. First of all, groundwater reservoirs can be divided in a finite number of layers. This is called layered heterogeneity. Every layer has its own sedimentological characteristics (depositional structures, grain sizes, compaction, etc). From an hydrogeological point of view, permeable (pervious) and semi-permeable (semi-pervious) layers are defined. These are relative terms. A silty deposit can be considered as permeable in one groundwater reservoir while in another it can be considered as semi-permeable. Impermeable (impervious) layers are a purely theoretical concept and are only used for modelling purpose. No layer found in nature is completely impervious. Secondly, layers are not internally homogeneous. Sedimentological structures are present and they can vary laterally. Every depositional environment has its own sedimentological characteristics and both layered and lateral variation occur within layers. So, within a layer additional layered and lateral heterogeneity occur.

Three main classes of heterogeneities can be considered. In sedimentary rocks there is usually a layered heterogeneity. The individual bed of a geological formation can be considered as being more or less homogeneous at a small scale but each bed has a different hydraulic properties. Also typical for sedimentary rocks is the trending heterogeneity which is related to sedimentary processes. Discontinuous heterogeneity can be caused by the presence of faults, sudden facies changes, etc.

With the aid of drillings the spatial structure of layers can be studied. If many drilling descriptions are available, one can have an idea about the large scale lateral variation in individual layers. However, drillings are costly and more limited information is in most cases present than one would wish. Additional information on large scale structures but also on small scale structures can be found in quarries and outcrops. Although an idea about heterogeneity even on different scale can be formed, the
issue stays what the effect on hydraulic parameters is and how to deal with it in practical application (for instance in groundwater modelling).

3.2 Hydraulic Parameters in Heterogeneous Aquifers

3.2.1 Hydraulic conductivity

Because the way geological units are deposited, hydraulic conductivity will vary from place to place. If N conductivity measurements are available in a unit, a histogram can be made. It is now generally accepted that the probability density distribution for the hydraulic conductivity is log-normal (or natural logarithm) (Domenico & Schwartz, 1998). A log-normal distribution for K is one for which a parameter Y, defined as $Y = \log(K)$ (or $Y = \ln(K)$), shows a normal distribution. In a geological unit, a sample mean $Y_m$ and variance $S_Y^2$ can thus be found representing the real mean hydraulic conductivity $µ_Y$ and variance $\sigma_Y^2$. These are characteristics of the unit. Following Freeze & Cherry (1979) the standard deviation on Y is usually in the range of 0.5-1.5. This means that the K-values in most geological formations show internal heterogeneous variations of one to two orders of magnitude.

Hydraulic conductivities do not occur totally at random. Values measured quite close to each other are less different than values measured far apart. Values measured close to each other are thus stronger correlated. Therefore, a correlation length is defined. This is a measure of the spatial persistence of zones of similar properties. Variograms\(^1\) are a very useful tool in the description of spatial structures and function of conductivity. Consider N measurements $z(x_1)$, $z(x_2)$, … $z(x_N)$. The $x$ stands for the array of coordinates of the point where these measurements were taken. The variogram is the plot of the square difference $\gamma(h) = 1/2 \left[ z(x_i) - z(x_j) \right]^2$ against the separation distance $h = \| x_i - x_j \|$. A variogram is stationary if for large separation distances $h$, it reaches constant $\gamma(h)$. On a variogram, the correlation length is the length scale at which the sill is obtained. The sill is the value around which the stationary variogram stabilises. The correlation scale is also a characteristic of the unit. The correlation scale can be the same in all directions. In reality, the vertical correlation length is almost always found to be smaller than the horizontal correlation length.

To summarise, the statistical description of hydraulic conductivity of a geological unit can be described statistically with a mean, variance and correlation length. If the unit is anisotropic, these vary in function of the direction of measurement. The horizontal conductivity is in most cases larger than the vertical conductivity. The unit is statistically anisotropic when the mean, variance and correlation length vary according to the direction. It is also possible to describe hydraulic conductivity in more complex random fields, for instance in situations were there is a trend (for instance the mean increases in one direction) (Deutsch & Journel, 1998).

What about conductivity anisotropy, this is the ratio of horizontal to vertical conductivity? It is expected that anisotropy will increase with heterogeneity. Some calculations have been performed to illustrate this. Take in consideration a geological unit with layered heterogeneity. The resulting horizontal and vertical hydraulic conductivity of the combination of these layers also called the equivalent horizontal hydraulic conductivity $K_h$ and vertical hydraulic conductivity $K_v$ are (Lebbe, 1999a):

\(^1\) Mathematical treatment of variograms can be found in for instance Kitanidis (1997) or Deutsch & Journel (1998).
\[ K_h = \sum K_{hi} f_i \quad \text{and} \quad \frac{1}{K_v} = \sum \frac{f_i}{K_{vi}} \] 3.1

Where \( K_{hi} \) and \( K_{vi} \) are the horizontal and vertical conductivity of the individual layers and \( f_i \) is ratio of the thickness of the \( i^{th} \) layer to the total thickness of all layers. If one assumes that the hydraulic conductivities of the individual layers also show a log-normal distribution and that each layer behaves as an isotropic unit, one can calculate the equivalent horizontal and vertical conductivity of this formation with equation 3.1. If the whole log-normal distribution is considered then the result is that the equivalent horizontal conductivity is always infinitely large and the equivalent vertical conductivity is always infinitely small. Therefore, only meaningful values for the equivalent horizontal and vertical conductivities are obtained when only the central part of the log-normal distribution is considered while the tails are ignored. Figure 3.1 shows the relation between equivalent anisotropy \((K_h/K_v)^{1/2}\) and the standard deviation of the log-normal distribution for different central parts of the log-normal distribution taken into consideration. From such calculations, some important conclusions with regard to modelling in heterogeneous aquifers are drawn:

- The mean of the log-normal distribution is always equal to the equivalent effective conductivity of the layered formation or \((K_h K_v)^{1/2}\)
- When the heterogeneity increases (increase of the standard deviation of the log-normal distribution) then the equivalent anisotropy of the layered formation increases.
- The equivalent anisotropy is strongly dependent on the considered central part of the log-normal distribution. When more distal parts of the distributions (in a certain sense the outliers) are considered, the anisotropy becomes larger.

![Figure 3.1 Relation between equivalent anisotropy \((K_h/K_v)^{1/2}\) and the standard deviation of the log-normal distribution for different central parts of the log-normal distribution (Lebbe, 1999a).](image)

3.2.2 Specific Elastic Storage

Specific elastic storages are important in the beginning of the pumpage during a pumping or forced gradient tracer test. It is of less importance for solute transport. In larger regional transient groundwater flow models, values of specific elastic storage and storage coefficients near the water table must be assigned. However, no literature is known to the author which studies the distribution of these values in groundwater reservoirs.
3.3 Solute transport Parameters in Heterogeneous Aquifers

3.3.1 Dispersivity

Dispersivity values tend to be dependent on the scale of the observation. This has been derived from numerous field studies on dispersivity. Summaries are provided by Anderson (1979, 1984) and Gelhar et al. (1985, 1992). The form of the dependency is, however, less certain (e.g. Pickens & Grisak, 1981; Molz et al., 1983; Neuman, 1990). Gelhar et al. (1992) have put available tracer test data in function of scale (figure 3.2), clearly indicating an increasing trend in dispersivity with increasing scale. These authors, however, suggest not only to look at the dispersivity test data, but also to take into consideration the reliability with which the data are obtained. They use therefore three classes based on predefined criteria: low, intermediate and high reliability. They argue that there are a wide range of aquifer types and different test by which the results were obtained. Now looking only at the high reliability data, a trend is less apparent. Note in this context that all high reliability data are based on small scale tests, so there is definitely a need on reliable values derived on larger scales.

![Figure 3.2 Longitudinal and lateral dispersivity in function of scale (Gelhar et al., 1992).](image)

Although many questions remain, some general conclusions can be derived from the work of Gelhar et al (1985, 1992):
Dispersivity tends to increase with scale. Some stochastic theories predict an asymptotic approach to a constant dispersivity value with increasing scale of observation. Based on figure 3.2, it is not clear which value this asymptotic dispersivity has.

For a given scale, the dispersivity range over two to three orders of magnitude. This illustrates that the derived value is highly dependent on the aquifer material and internal structure (see further). The most reliable data fall in the lower portion of this range.

Transverse dispersivity is generally smaller than longitudinal dispersivity and tends to be also scale dependent. However, ratio between longitudinal and transverse dispersivity is mostly set by scholars at a certain ratio (e.g. 3 or 10 times). If looking therefore only at reliable data, a trend is less certain. This is the case for both horizontal and vertical transverse dispersivity.

Longitudinal dispersivity is generally larger than transverse dispersivity and horizontal transverse dispersivity is generally larger than vertical transverse dispersivity. High reliability data indicate that the ratio between longitudinal and horizontal transverse dispersivity is in the order of 10. The vertical transverse dispersivity is two to three orders of magnitude smaller than the longitudinal dispersivity.

Figure 3.2 is often used as an indication of which dispersivity values to use in field applications and modelling. Gelhar et al. (1992) themselves, however, warn about this. They argue that derivation of an ‘universal’ scaling trend (or at the end, a formula giving dispersivity in function of scale) is impossible because every aquifer is unique. The type of problem one is dealing with will also determine the dispersivity values. In the past, some attempts have been made to make scaling formulas (e.g. Peaudecerf & Sauty, 1978; Sudicky & Cherry, 1979; Pickens & Grisak, 1981; Arya, 1986; Neuman, 1990; Xu & Eckstein, 1995). In these cases, dispersivity has been treated as a function of travel distance of the tracer and linear as well as parabolic, asymptotic and exponential relations have been sought. At best, relations are only valuable within certain scale limits in one particular aquifer for which they are derived. Figure 3.3 shows some of these relationships with the data set of Gelhar et al. (1992). Obviously, no ‘universal’ relationship has yet been developed.

**Figure 3.3** Some relationships of longitudinal dispersivity in function of scale compared with the data set of Gelhar et al. (1992).

Why does dispersivity tend to increase with scale? In Chapter 2, it has been shown that microscopic dispersion is the result of departures of the actual flow velocity from the calculated seepage velocity
due to microscopic heterogeneity and tortuosity of a granular porous medium. The resultant dispersivities are very limited, longitudinal dispersivity is in the order of 0.01-1.00 cm. Dispersion on the field scale is caused primarily by macroscopic heterogeneities rather than pore-scale heterogeneities, hence the larger values. Hydraulic parameters vary between and in hydrogeological units. Depending on depositional and sedimentological conditions, these variations can be smooth, abrupt, layered, etc. The velocity field used in advective calculations (analytical or numerical) will be a smoothly varying function throughout the problem domain. Using for instance numerical methods, the velocity is calculated in nodes in the domain. It is considered that the hydraulic parameters (and hence also the velocities) are constant over an area (or volume) surrounding these nodes. The result is that the seepage velocity at best represents the average seepage velocity over that area (or volume) but that small velocity changes in it are not simulated. These small, but macroscopic velocity changes are responsible for the dispersion of the tracer. Because all these small velocity changes can not be included in a model, a dispersive component is needed besides the advective transport. Dispersivity can is this context be seen as a safety net for the modellers lack of knowledge and/or possibility to deal exactly with heterogeneity. Let's illustrate this with an example. Consider that we have two groundwater flow models describing the same problem. Model A, however, has two times more nodes than model B and therefore, the variation in hydraulic conductivity could be better represented in model A. All other things (schematisation, boundary conditions, stresses, etc) are the same. Because variations in hydraulic conductivity could be better implemented in model A, the dispersivity needed to simulate solute spreading will be smaller than in model B. However, this illustrates the need to have detailed information on heterogeneity and hydraulic and solute transport parameters over the whole model domain, something which is never the case. Additionally, model A is a larger model and will need more computer time. Although desk top computers become more powerful every day, there is obviously a practical limit on the duration computer models can be run. If we should have complete knowledge of heterogeneity and parameter values in the model domain, could represent all boundary and stress conditions properly and have a powerful computer to use, the model should be simulate solute transport only by calculating advective transport. So, dispersivity used in numerical models, not considering numerical dispersion, is due to three causes:

1. Used hydraulic and solute transport parameters are averaged over the model cell. No smaller scale variations than the cell dimensions can be implemented. Heterogeneity in hydraulic conductivity attributes most to dispersivity due to the gaussian log-normal (or ln) distribution in hydrogeological units.
2. Our field knowledge about site heterogeneity and parameter values is limited because of the limited observation points. So, on basis of the limited knowledge we do have in a region, a model is constructed, smoothing out heterogeneities and variations in parameter values.
3. Due to limited computer time, number of nodes or elements is limited. Less nodes or elements mean that parameters are averaged over larger areas or volumes.

Observations made by Gelhar et al. (1992) (figure 3.2) can now be explained. First of all, dispersivity tends to increase with scale. The farther a tracer plume has travelled, the more velocity changes it will have undergone and the more dispersed it will be. This is modelled with cells with average valued parameters. Thus, the longer the plumes travel distance, the more velocity variations which will be smoothed in the model resulting in larger dispersivity which will be needed. Solute transport is for instance modelled as Fickian. This means that the departures of actual particles velocities from the advective velocities are in all directions the same. Although this is a reasonable assumption on pore scale, this comes into question on larger scales. If heterogeneity within one cell is dominated by a few major features, the departures may be biased toward a particular direction. The flow is thus not Fickian. Over a large number of elements, effects of this kind would tend to cancel and the calculations based on the Fickian model will go to an asymptotic value. Before this asymptotic value is reached, dispersivity based on the Fickian model will grow with scale.

For a given scale, the dispersivity range over two to three orders of magnitude. This is due to specific aquifer properties and model characteristics. The larger the heterogeneity, the larger the dispersivity will be. Even so, the larger the cells the larger the dispersivity will be.
The dispersivity resulting from the macroscopic heterogeneity is called the macroscopic dispersivity or macrodispersivity. Describing and identifying this macrodispersivity is still topic of ongoing research. Some of the most early contributions are those of Gelhar et al. (1979), Matheron and de Marsily (1980), Dagan (1982a,b 1984), Cushman (1983), Gelhar and Axness (1983), Wheatcraft and Tyler (1988), Neuman (1990) and Neuman and Zhang (1990). Most recent contributions are summarised in Dagan and Neuman (1997) and Zhang (2001). The most active line of research has focused on stochastic approaches. Hydraulic conductivity is considered as a random variable and generates a dispersive effect in the calculated solute concentration. Depending on the assumptions that are made regarding the hydraulic conductivity distribution, the dispersive effect may or may not turn out to be similar to diffusion as calculated by Fick’s law. A number of stochastic models predict that the diffusive model will be asymptotically, and that macroscopic dispersivity will approach a constant value as the distance of transport becomes large. Stochastic theories dealing with dispersivity generally relate scaling effects to increases in spatial variability of hydraulic conductivity with distance (Dagan, 1982b, 1984; Gelhar & Axness, 1983). They also predict that dispersivity should approach a constant value as the hydraulic conductivity becomes statistically uncorrelated at increased distances, that is, as the scale of an equivalent homogeneous medium is reached. Other approaches have focused on volume averaging (e.g. Plumb & Whitaker, 1988). Equations are developed in terms of average values of concentration and velocity over volumes of the aquifer that incorporate macroscopic heterogeneities. Again, depending on the nature and scale of the heterogeneities and the scale at which the volume averaging is done, the resulting description of macrodispersive transport may or may not approximate the diffusion model.

Although there is discussion when dispersivity, before an asymptotic value has been reached, obeys Fick’s law, it is generally accepted that solute transport under macroscopic conditions is best simulated with the Fickian model. At present, most of the transport simulation codes treat dispersion as obeying the diffusive model. This is a good approximation as long as the scale of the heterogeneities is small, relative to the distance of transport or scale of calculations.

These conclusions explain the observations by Tiedeman & Hsiew (2002). They have shown by theoretical numerical modelling that the value of longitudinal dispersivity is also affected by the type of test with which it is derived. These authors simulated the derivation of dispersivity in a two dimensional aquifer with different tests. Heterogeneous aquifers were generated according to a spherical variogram. Converging radial-flow, two-well tracer tests and large scale natural gradient tracer tests were simulated in two-dimensional aquifers. Longitudinal dispersivity estimates in mildly heterogeneous aquifers ($\sigma^2_{\ln(k)}=1$) and with long transport distances were generally similar for the radial-flow and two-well tracer tests. These values equalled the results of a large scale natural gradient tracer test in the same aquifer. In highly heterogeneous aquifers ($\sigma^2_{\ln(k)}=6$), estimates from two-well tests are generally larger than those from radial-flow tests. Natural gradient tracer tests derived the largest values. For small separation distances, the estimates from the two-well tests spanned a wide range of values but were generally larger than those from the radial-flow tests. These results are explained by looking at the volume of aquifer sampled by the tracer. In a converging radial-flow test, the tracer samples a relatively narrow volume of aquifer between the injection and pumping well. This volume is considerably larger during a two-well tracer test. The relation between volume of aquifer sampled by the test, heterogeneity ($\sigma^2_{\ln(k)}$) and separation distance stipulate the outcome. For instance, values derived with different test may be approximately the same in a highly heterogeneous aquifer but with very small separation distances because an asymptotic dispersivity value is already reached. This asymptotic value is then derived with all tests. A larger separation distance and mildly heterogeneous aquifer may provide different dispersivity values for different tests since the asymptotic value is not yet reached. The derived value is then result of aquifer volume sampled and travel distance.
3.3.2 Porosity

Porosity $n$ is the percentage of rock or sediment that is void of material. The effective porosity $n_e$ is the porosity available for fluid flow. Porosity and effective porosity are more or less the same for sandy sediments. The pores are interconnected fluid pathways. In clay sediments, effective porosity is usually smaller than the porosity because of an important amount of dead-end pores. Porosity is important in two ways concerning solute transport. It is a factor in defining seepage velocities controlling advection and it is used in dispersion. Secondly, it determines the pore volume of a model cell available for storage of solute mass.

Porosity values from a single unit tend to have normal, rather than log-normal distributions. Some relations between porosity and sedimentological characteristics are known. Principally, two types of relations can be distinguished. The first type is based on grain size diameter. The second type is based on the specific surface of sand and part of the silt fraction.

Equation 3.2 gives an example of a relationship between grain sizes and porosity via sorting. Porosity is strongly correlated with sorting. When sorting increases, so does porosity. This is given in a relationship by Scherer (1987):

$$n = 20.91 + \frac{22.9}{S}$$  

3.2

where $S = 2^z$ and $z = \frac{(\phi_{75} - \phi_{25})}{2}$

$S$ is the sorting expressed in phi quartiles given in $z$. 

32
4.1 Selection of an appropriate test

4.1.1 Introduction

One of the aims of this research is the derivation of reliable hydraulic and solute transport parameters. This is accomplished through the design of tests from which these parameters can be deduced. In chapter 2, an overview is provided of frequently used tests. Basically, these can be divided into three categories from a scale point of view: small scale tests, field scale tests and regional scale tests. Small scale tests are the laboratory tests, like permeameter tests, column experiments, etc. Disadvantage of this kind of tests is the small volume of aquifer material that is used. This leads to upscaling problems as discussed in chapter 3 questioning the usability of the parameters on large scale applications. Field scale tests are performed under field circumstances. They include pumping tests, tracer tests, etc. The aquifer is tested on a scale of ten to maximum hundred metres. Larger tests are regional or large scale tests, such as tracer tests with natural occurring tracers or large contamination plumes.

In this wealth of tests, field scale test provides some advantages:

- It is a field test and processes are studied on the scale as they occur on the field. Further, the volume of aquifer one is studying is minimally disturbed. This is in contrast with laboratory tests where small samples of disturbed material are used.
- The scale of the test is also not too large meaning that the test is done under more or less strictly known and controllable spatial boundary conditions. In large regional tests, boundary conditions are far less accurately known.
- If pumpages are used, duration of the test is relatively small, in the order of 10 to 14 days for tracer tests for instance. This eliminates the difficulty to accurately monitoring and modelling natural occurring time dependent phenomena such as recharge, discharge, varying natural gradients, etc.

4.1.2 Forced gradient tracer test

Pumping tests and tracer tests are field tests and both have their advantages and disadvantages. With a pumping test, drawdown measurements are used to derive hydraulic parameters from pumped and adjacent layers. The derived parameters are layer averages, for instance the hydraulic conductivity of
the pumped layer. The parameters are derived on field scale and can more readily be used in larger regional models than laboratory tests. With the interpretation method for pumping tests that will be used here (Lebbe, 1999a), detailed vertical heterogeneity of the groundwater reservoir can be implemented in the model. However, no information about lateral variation of hydraulic parameters and fine scale vertical heterogeneity can be deduced.

With a tracer test, concentration observations are used to derive travel times and dispersion of a tracer. Seepage velocities determine the travel times when only advection and dispersion (no chemical reactions) are considered. As discussed in chapter 2, seepage velocity $v$ equals $(K_i)/n_e$. The hydraulic gradient $i$ can be measured on the field with observation wells and from concentration observations, seepage velocities can be determined. With the seepage velocity and hydraulic gradient, the ratio of hydraulic conductivity to effective porosity is known. To derive the hydraulic conductivity of the layer in which the tracer moves, one has to know its effective porosity. In other words, to match the concentration of the tracer test, one has to ‘play’ with the ratio $K/n_e$ and no reliable value of either of them can be deduced.

![Figure 4.1 A forced gradient test starts with the injection of a tracer. Then water is extracted from the pumping well. The movement of the tracer is followed with observation wells between the injection and pumping well. Screened sections are indicated.](image)

So, both tests have their strong points and their set-backs. The idea behind a forced gradient tracer test is to eliminate the set-backs by combining the strong points. A forced gradient tracer test consists of two steps. First, a volume of water marked with a tracer is injected in the groundwater reservoir. Thereafter, pumping is started on a well, placed at a certain distance from the injection well. The movement of the tracer towards the pumping well is monitored with observation wells between the injection and pumping well. Typical distances between the two wells are 5 to 10 metres. During the pumping phase both concentration and drawdown observations can be made. Dispersivity and effective porosity can be derived from the concentration observations, specific elastic storage from the drawdown observations and hydraulic conductivity from both the drawdown and concentration observations.
observations. First, hydraulic conductivity is derived from the drawdown observations. This conductivity is a bulk conductivity of for instance the pumped layer. This value is used to model the tracer test and derive effective porosity from concentration observations. Conductivity of smaller horizons can be determined using the concentration observations. It may be, and in most cases will be, appropriate to reconsider the drawdown interpretation based on new information gained from the concentration observations. After a few of such iterations, hydraulic conductivity used to model the concentration and drawdown observations must be in agreement, taking into account the fact that with a tracer test hydraulic conductivity of smaller horizons can be studied than with a pumping test. The statements made here will be thoroughly tested with data collected on three field site in chapter 5.

4.1.3 Type of tracer and method of observation

The type of tracer and the method of observation used during the forced gradient tracer test are for obvious reasons closely related. Aim of the forced gradient tracer test performed here is to study advection and dispersion in the porous medium. No chemical or (micro)biological reactions are desirable because this complices the interpretation of data considerably. Therefore, a conservative tracer is needed. As conservative tracer, we opted for salt water. This choice is closely linked with the method of observation. Ideally, tracer breakthrough can be studied in detail in different observation wells and on different levels. Water samples are only a crude way to do this because they are the net result of the water quality over a relatively large depth interval. Additionally, when samples on different horizons in one observation well are taken, long screens must be used. This raises the risk of hydraulic short-circuiting considerably introducing errors in the data set. Optimally, concentration observation in continuos vertical profiles between injection and pumping well should be available. With the use of salt water and geophysical borehole measurements, this is possible.

The movement of the tracer plume is followed with geophysical borehole logs. Salt water has a higher electrical conductivity than fresh water. When salt water is present in the vicinity of an observation well, the electrical conductivity around this well will be large. For this research we used a focused electromagnetic induction tool (EM39) of Geonics Limited. The EM39 is specifically designed for use in plastic-encased wells. EM39 employs a small internal transmitter coil energised with an audio-frequency current to induce eddy currents in the soil surrounding the well. These eddy currents generate an alternating secondary magnetic field which can be detected and measured by a small receiver coil located some distance away from the transmitter. The small secondary magnetic field will be essentially linearly proportional to the electrical conductivity of the surrounding material and the device can be calibrated to read the terrain conductivity directly (McNeill, 1986). Distance between transmitter and receiver coil is 50 cm. With this relatively short intercoil spacing, a centrally located focussing coil must be incorporated to reduce the response from conductive borehole fluid to negligible proportions. This arrangement of coils provides relatively large lateral range and a high degree of vertical resolution which makes it very suitable for hydrogeological research.

The relative response with radial distance from the well axis resulting from the coil configuration is shown in figure 4.2. The instrument is sensitive from a distance of 10 cm to 100 cm from the well axis with the most sensitive zone at a distance of 30 cm from the well axis. The instrument is therefore blind for the conductivity of fluids in the observation well and the disturbance around it. The vertical response of the instrument is also shown in figure 4.2. From this relative response graphs, it can thus be concluded that the electrical resistivity is measured in a torus centred around the observation well. The instrument is first order calibrated. A second-order correction is required for conductivities above 300 mS/m.
With the EM39 detailed vertical profiles can be made in observation wells during the tracer test. Different horizons of tracer breakthrough can therefore be observed. Typically, observations are made with an interval of 20 cm. This is of course a huge advantage in comparison with water samples as observation methods during tracer tests.

4.1.4 EM39 conductivity and total dissolved solids

Electrical conductivity can be recalculated in total dissolved solids (TDS, mg/l) in a straightforward way. Measurements with EM39 can therefore be recalculated in water qualities. The bulk resistivity ($\rho_b$, $\Omega$ m) of sediments is the combination of the resistivity of the sediment matrix ($\rho_m$, $\Omega$ m) and the resistivity of the pore water ($\rho_w$, $\Omega$ m):

$$\frac{1}{\rho_b} = \frac{1}{\rho_m} + \frac{1}{F \rho_w}$$

4.1

F ($) is called the formation factor. The pore water resistivity is function of TDS. The matrix resistivity is due to the presence of conductive (clay) minerals. If these minerals are scarce, for instance in sandy deposits, then the matrix resistivity becomes very large and the above relation becomes:
This is also known as Archie’s law (1942). Lebbe and Pede (1988) derived a relationship between the pore water resistivity and the TDS (mg/l) at 11°C:

\[ TDS = \frac{10000}{\rho_w} \quad \text{or} \quad TDS = F \frac{10000}{\rho_w} \]

As resistivity is related to conductivity (conductivity(\(\mu\text{S/cm)} = 10000/\text{resistivity(}\Omega\text{m)})) the electrical conductivity \(\sigma_b\) (mS/m) measured with the EM39 can easily be related to the total dissolved solids (mg/l) (Van Meir & Lebbe, 2002):

\[ TDS = 10F\sigma_b \]

With the above equation the EM39 conductivities can thus be recalculated to TDS values. This is the mean TDS value which is present in the observation torus according to the relative responses shown in figure 4.2.

### 4.2 Pumping test analyses

#### 4.2.1 Analytical solutions

Many analytical solutions to interpret pumping tests are available in literature. Lebbe (1999a) gives an overview of the most used interpretation methods. They are derived from models which consider simple groundwater reservoir schematisation with stringent boundary conditions. Some of the most used analytical models (model of Theis, Jacob-Hantush, Hantush and Boulton-Cooley) and their limitations are briefly discussed in section 2.6.2.

![Figure 4.3](image_url)

**Figure 4.3** The \((I,J)\text{th}\) ring and the surrounding rings of the axisymmetric grid used in HYPARIDEN. \(R_1\) is the initial radius and \(A\) is a factor which is larger than 1, mostly \(10^4\).
4.2.2 HYPARIDEN: a model package for pumping test analyses

HYPARIDEN (HYdraulic PARameter IDENTification) (Lebbe, 1999a), is a set of computer codes developed as a generalised interpretation method for single and multiple pumping tests. It is based on an axial-symmetrical model. The groundwater reservoir is subdivided in a large number of layers, each characterised by horizontal conductivity, a specific elastic storage and a value for the hydraulic resistance between different layers. The hydraulic resistance of a layer is its thickness divided by its vertical conductivity. In this way layered heterogeneity can be treated very accurately. Layers are laterally homogeneous and of very large extension. The layers are subdivided in a number of coaxial rings around the pumping well. In each coaxial ring a nodal point is considered for which calculations of drawdowns are done. This nodal point is at half height of the ring and its radius is equal to the geometric mean of the inner and the outer radius of the ring. The inner and the outer radii of the rings form a logarithmic series. Drawdowns are therefore calculated very accurately close to the pumping well where the largest and most important drawdowns occur. The groundwater reservoir is bounded on top by the water table, characterised by a storage coefficient near the water table, also called the specific yield. An impermeable layer is considered as lower boundary of the groundwater reservoir. The axial-symmetric nodal configuration is a major advantage (accuracy near the well as well as computing time) over current numerical groundwater flow models, e.g. MODFLOW, for pumping test simulation and analyses.

HYPARIDEN includes also an inverse numerical model allowing the derivation of optimal values for hydraulic parameters or hydraulic parameters groups. One such group may exist for instance of the horizontal conductivities of the different layers in which one semi-permeable layer is subdivided. All observations from different observation wells are involved together in the parameter identification process. The inverse model is a combination of a forward model, sensitivity analyses and a non-linear regression algorithm. With the residuals and the sensitivity analyses, adjustment factors of the most sensitive parameters are calculated after which these parameters are adjusted. This scheme is repeated until the adjustment factors become very small and the object function does not further reduce.

The forward numerical model calculates drawdowns on the nodes based on groundwater reservoir schematisation in different layers and with estimated hydraulic parameters for each layer. By interpolation between these nodal values, the drawdowns on observation places and times are calculated. With the observed (s*) and the calculated (s) drawdowns, residuals (r) are determined:

\[
    r = \log_{10}s^* - \log_{10}s
\]

The sum of squared residuals is the object function. Sensitivities are thereafter calculated. These are the changes in calculated drawdowns when one hydraulic parameter or parameter group is changed. If for instance one wishes to derive three parameters or group of parameters, one has to perform three sensitivity analyses. The sensitivity \( J_{ij} \) of the drawdown \( s_i \) to the hydraulic parameter or group of parameters, \( H_j \), is here approximated by the finite-difference method in which the drawdowns and the hydraulic parameters are considered in their logarithmic space:

\[
    J_{ij} = \frac{\log_{10}s_i(H_j*sf) - \log_{10}s_i}{\log_{10}sf}
\]

where \( sf \) is the sensitivity factor, \( s_i \) the calculated drawdown at the place and time of the \( i^{th} \) observation with the estimated values of the parameters during the first iteration or calculated values of the preceding iteration, \( s_i(H_j*sf) \) is the calculated drawdown at the place and time of the \( i^{th} \) observation with the estimated values of the parameters except for the values of the \( j^{th} \) parameter or group of parameters of which the estimated value(s) is (are) multiplied by the sensitivity factor.

By means of the linearization method (Draper & Smith, 1981) adjustment factors can be computed for hydraulic parameters or parameter groups so that the object function is minimised:
Chapter 4: Parameter Identification Tests

A. Vandenbohede

\[ A = (J^T wJ)^{-1} J^T w r \] \hspace{1cm} (4.7)

Where \( A \) is the vector of the logarithms of the adjustment factors of the different parameters and \( J \) is the matrix of the sensitivity coefficients or the Jacobian. \( J^T wJ \) is called the Hessian matrix. The objective function that is to be minimised, is the weighted square of the residuals:

\[ S = \sum_{i=1}^{n} w_i r_i^2 \] \hspace{1cm} (4.8)

where \( n \) is the number of observations, \( w_i \) is the weight of the \( i \)th observation and \( r_i \) is the residual of the \( i \)th observation. In the ordinary least square method (OLS) all the weights are equal to one. In the weighted least square method (WLS) every observation has a weight. The used WLS is the biweighted least square method (BWLS) (Wonnacott and Wonnacott, 1985). In this method, a kind of standardised residual is calculated:

\[ u = \frac{r}{3IQR} \] \hspace{1cm} (4.9)

where IQR is the interquartile range of the residuals or the distance between the lower and upper quartiles of the residuals. The lower and upper quartiles correspond with a cumulated frequency or probability of 25\% and 75\%. The weight is now given in a diagonal matrix \( w \) where the weight of the \( i \)th observation is given in the diagonal element \( w_{ii} \):

\[ w_{ii} = (1-u_i^2)^2 \quad \text{if} \quad |u_i| \leq 1 \] \hspace{1cm} (4.10)

\[ w_{ii} = 0 \quad \text{if} \quad |u_i| > 1 \]

New estimated values of the parameters are obtained by adding the logarithms of the adjustment factors to the corresponding logarithmic values of the \( j \)th parameter of the former iteration or:

\[ h_{pj}^{m+1} = h_{pj}^m + A_{pj}^m \] \hspace{1cm} (4.11)

where \( h_{pj}^m \) is the logarithmic value of the \( j \)th parameter during the \( m \)th iteration of the inverse process and \( A_{pj}^m \) is the logarithm in base 10 of adjustment factor of the \( j \)th parameter calculated after the \( m \)th iteration.

Usually it is impossible to include all the deducible parameters at the start of the iteration process. When very sensitive parameters are included along with much less sensitive parameters in the iteration process, it happens that the Hessian matrix is not well conditioned. This results in unreliable values for the adjustment factors. The smaller the sensitivities of the parameters the less reliable their adjustment factors are. To overcome this problem, it is advisable to introduce first the most sensitive parameters in the iterative process. The minimisation process is then continued until it converges to an optimum solution with this limited number of hydraulic parameters. Then other parameters can successively be included according to the order of magnitude of their sensitivities.

The result of the inverse model is the optimal values of the hydraulic parameters or parameter groups and some statistical parameters which characterise the joint confidence region. This joint confidence region of the statistical parameters informs about the accuracy with which these parameters are deduced from the observations.

When the assumption that the residuals exhibit a normal distribution is not violated as well as the assumption that the drawdowns can be approximated as a linear function within the considered region
then the joint confidence region can be described by the optimal values and the variance-covariance matrix of the parameters $\text{cov}_p$:

$$
\text{cov}_p = \sigma_s^2 (J^T w J)^{-1}
$$

where

$$
\sigma_s^2 = \left( \sum_{i=1}^n r_i^2 \right) / (n-p)
$$

$n$ is the number of observations and $p$ the number of parameters. The marginal standard deviation $s_m$ of the $j^{th}$ parameter is the square root of the $j^{th}$ diagonal term of the covariance matrix (Carrera and Neuman, 1986). The partial correlation coefficient between the parameters $p_j$ and $p_{j+1}$ is $\text{cov}_{j,j+1} / (s_m^j * s_m^{j+1})$. The conditional standard deviation $s_c$ of the $j^{th}$ parameter can be approximated using the eigenvalues and the eigenvectors of the covariance matrix (Lebbe, 1988):

$$
s_c = \left( \sum_{k=1}^p \beta_{jk}^2 / \alpha_k \right)^{-1/2}
$$

where $\alpha_k$ is the $k^{th}$ eigenvalue of the covariance matrix and $\beta_{jk}$ is the $j^{th}$ term of the $k^{th}$ eigenvector of the covariance matrix.

According to Belsley (1990) the marginal variance of the $j^{th}$ parameter

$$
\text{var}_m = \sigma_s^2 \sum_{k=1}^p \var_j^2 / \mu_k^2
$$

where $\mu_j$ is the $j^{th}$ singular value of the sensitivity matrix $J$ and $\var_j$ is the $j^{th}$ term of the $k^{th}$ eigenvector of the Hessian matrix $J^T J$. The proportion of the marginal variance of the parameter $p_j$ associated with the $k^{th}$ singular value is given by:

$$
\pi_{jk} = \var_j / \var_j \\
\var_j = \beta_{jk}^2 / \mu_k^2 \\
\mu_k = \sum_{k=1}^p \var_k
$$

The proportion is associated with a condition index $\eta_k$, which is the ratio of the largest singular value ($\mu_{\text{max}}$) to the singular value $\mu_k$. The largest value of $\eta_k$ is called the condition number of the problem. Weak dependencies between parameters are associated with condition indexes around 5 to 10, whereas moderate to strong dependencies are associated with condition indexes of 30 to 100 (Belsley, 1990).

### 4.3 TRACER3D: numerical model for tracer test analyses

#### 4.3.1 TRACER3D program package

TRACER3D is a program package to simulate numerically, three-dimensional density dependent solute transport in the vicinity of pumping wells. Several numerical models already exist which can model in 3D solute transport, so why make another one. Several reasons can be quoted:

- The flow of salt water is to be modelled, hence the flow is density dependent. Modelling of density dependent flow has its own inherent difficulties and therefore, not many 3D codes exist. MOCDENS3D (Oude Essink, 1998) is a notable exception.
- Running a 3D groundwater flow model can be a (computer) time consuming occupation, especially when pumping wells come into play. This is both due to the transient flow around a pumping well and the computing accuracy which is necessary. Head is changing in function of time and distance from the pumping well. The most rapid and largest changes occur close to the well. Therefore, small cell sizes in the numerical model must be used. This of course increases the number of cells drastically and moreover, a lot of computing power is wasted in model region where this accuracy is not needed.

Conclusion is therefore that existing computer codes, although perfectly capable from a theoretical point of view, are totally unsuitable from a practical point of view to model solute transport accurately enough around a pumping well. A novel approach to this problem is used here in TRACER3D:
• First of all, the drawdowns in function of time and distance from the pumping well are calculated using the two-dimensional forward pumping test simulation model taken from the HYPARIDEN package.
• The model area is a box, centred around the pumping, injection and observation wells (figure 4.4, box 1). The same assumptions used in HYPARIDEN are valid. The groundwater reservoir is subdivided in a large number of layers, so layered heterogeneity is accounted for. Every layer is characterised by a value for the horizontal hydraulic conductivity, specific elastic storage and hydraulic resistance. Drawdowns in this 3D grid are calculated as function of distance from the pumping well and time. HYPARIDEN is a 2D model but the calculated drawdowns can be extrapolated axi-symmetrical in 3D. Lines of equal drawdowns are concentric circles around the pumping well. This means that the drawdowns calculated in HYPARIDEN can be used as input. Lateral heterogeneity is not accounted for.
• In the model area, a second box (figure 4.4 box 2) is considered around the injection well. Numerous particles are placed in this box. Every particle is characterised by its coordinates and a concentration (TDS). With these particles, the tracer plume can thus be modelled. Particles outside the tracer plume are given a background concentration. This background concentration can vary vertically in the reservoir. Therefore, layers with different background concentrations (here called concentration layers) can be incorporated. Transition zones between fresh and salt water for instance can thus be implemented. Particles can also be placed in box 1 or in a selected part of box 1. This is done for instance when the water quality varies in the groundwater reservoir. The interaction between the tracer plume and the natural occurring groundwater is then incorporated. The movement of the particles and the concentration changes are followed in time. Advection and dispersion are modelled with the method of characteristics MOC (Konikow & Bredehoeft, 1978).

![Figure 4.4 Model domain as used in TRACER3D.](image)

In this way, all the computing power is concentrated on the region of interest concerning the solute transport and the drawdowns are calculated very accurately where this has to be the case.

4.3.1.1 Calculation of advection and dispersion

Numerically solving the advection-dispersion equation provides some difficulties. Although advection and dispersion occur simultaneously, they promote mass transport very differently. Advection is mass transport along flow lines while dispersive transport is also occurring between flow lines. Mathematically, this means that simultaneously a hyperbolic (advection) and a parabolic (dispersion) equation must be solved. This is a problem that no numerical method has fully overcome yet.
One way of solving the advection-dispersion equation is using the method of characteristics (MOC). It is a mixed Eulerian-Lagrangian method. In Eulerian methods, the transport equation is solved in a fixed spatial grid. Finite-difference and finite-element methods are primary examples of this class of solution methods. They offer the advantage and convenience of a fixed grid, are generally mass conservative and handle dispersion-dominated problems both accurately and efficiently. However, advection dominated problems are susceptible to excessive numerical dispersion or artificial oscillation (Pinder & Gray, 1977; Andersen, 1979). In Lagrangian methods, the transport equation is not directly solved. A large number of moving particles are used to approximate both advection and dispersion. Lagrangian methods provide an accurate and efficient solution to advection dominated problems essentially eliminating numerical dispersion (e.g. Prickett et al., 1981; Kinzelbach, 1986; Tompson & Gelhar, 1990). However, the lack of a fixed grid or fixed coordinates can lead to numerical instability and computational difficulties. Velocity interpolation can also result in local mass-balance errors and solution anomalies (LaBolle et al., 1996).

Figure 4.5 A: Part of hypothetical finite-difference grid showing relation of the flow field to the movement of points. B: Part of hypothetical finite difference grid showing areas over which bilinear interpolation is used to compute the velocity at a point. Note that each area of influence is equal to one-half of the area of a cell (Konikow & Bredehoeft, 1978).

Lagrangian methods are thus particularly suitable for handling advection, while Eulerian methods are more effective in dealing with dispersion. The mixed Eulerian-Lagrangian approach attempts to take advantage of this fact by solving the advection term with a Lagrangian approach (particle tracking) and the dispersion and reaction terms with an Eulerian approach. The movement of a large number of particles is tracked and its concentration changes are calculated. The basic finite-difference algorithm is for the concentration change of cell m is:

$$C^{n+1}_m = C^n_m + \frac{DC}{Dt} \Delta t$$  \hspace{1cm} 4.15

$$\frac{DC}{Dt} = \nabla.(D \nabla C)$$  \hspace{1cm} 4.16
where \( C_{m}^{n+1} \) is the average solute concentration for cell \( m \) at new time level \( n+1 \) and \( C_{m}^{n*} \) is the average solute concentration for cell \( m \) at new time level \( n+1 \) due to advection alone. \( D \) is the dispersion coefficient, \( t \) is time and \( C \) is the concentration. The first part of equation 4.15 accounts for the effect of advection and is solved with a Lagrangian particle tracking method. The second term accounts for the effects of dispersion and is solved with a finite-difference method in fixed Eulerian grid.

First step in the modelling is the discretisation of the ground water reservoir in model layers. To enhance accuracy, the depth interval is divided in small layers, typical 20 to 30 cm thick. With this schematisation, the drawdowns are calculated in all these layers in function of distance from the pumping well and time with the forward model of HYPARIDEN. The result is written down on a separate file. This is the basis for further calculations.

The same schematisation of the groundwater reservoir is used for the simulation of the tracer test. In box 2 (and box 1 if necessary), a large number of particles is placed, typical with an in-between distance of 5 to 10 cm. Every particle is characterised by its coordinates in the model region and by a TDS value. Particles that do not make up the tracer plume, are given a background concentration. This background concentration can very with depth. The time that is to be modelled is divided in a number of time steps. This number is determined by stability criteria for the solute transport simulation, discussed further on. In every time step, the advective movement of all particles and the concentration changes due to dispersion are calculated.

![Figure 4.6 Representative change in breakthrough curve from time level \( k-1 \) to \( k \) (Konikow & Bredehoeft, 1978).](image)

The particle location at any time \( t \) can be expressed as:

\[
p(t) = p(t_0) + \int_{t_0}^{t} v(p, t) dt
\]

where \( p(t_0) \) is the position vector at time \( t_0 \), \( p(t) \) is the position vector at time \( t \) and \( v(p, t) \) is the seepage velocity vector. This equation can be solved by numerical integration. The simplest numerical
integration method is Euler’s method. This is used in the MOC method of Konikow and Bredehoeft (1978) applied here:

\[
\begin{align*}
x(t) &= x(t-1) + v_x \Delta t \\
y(t) &= y(t-1) + v_y \Delta t \\
z(t) &= z(t-1) + v_z \Delta t
\end{align*}
\]

where \(x(t-1), y(t-1)\) and \(z(t-1)\) represent the position of the particle at the end of time step \(t-1\), \(\Delta t\) is the duration of a time step and \(v_x, v_y\) and \(v_z\) are the seepage velocities in the \(x, y\) and \(z\) direction at time \(t-1\) and position \(x(t-1), y(t-1)\) and \(z(t-1)\). For Euler’s method to be accurate, the time step \(\Delta t\) must be sufficiently small. This is because the method uses only the velocity at the starting point of each step and this velocity is extrapolated over the whole time interval \(\Delta t\). Seepage velocities are:

\[
\begin{align*}
v_x &= \frac{K_{h,p} s_x - s_p}{n} \frac{\Delta x}{\rho_p - \rho_f} \\
v_y &= \frac{K_{h,p} s_y - s_p}{n} \frac{\Delta y}{\rho_p - \rho_f} \\
v_z &= \frac{K_{v,p} (s_z - s_p)}{n} \frac{\Delta z}{\rho_p - \rho_f}
\end{align*}
\]

where \(K_{h,p}\) and \(K_{v,p}\) are the horizontal and vertical hydraulic conductivity of the layer in which the particle moves; \(s_p\) is the drawdown at the initial position of the particle in time step \(t\); \(s_x, s_y\) and \(s_z\) are drawdowns on a distance \(\Delta x, \Delta y\) and \(\Delta z\) from the initial particle position in time step \(t\) in the \(x, y\) and \(z\) direction. The \(s, s_x, s_y\) and \(s_z\) are interpolated bilogarithmic in space and logarithmic in time from the drawdown file calculated in HYPARIDEN. The term \((\rho_p - \rho_f)/\rho_f\) is called the buoyancy and adjusts the vertical velocity for density effects. Density and concentration are linked by the equation of state:

\[
\rho_b = \rho_f \left(1 + \frac{\rho_b - \rho_f}{\rho_f} \frac{TDS_p}{TDS_s}\right)
\]

where \(TDS_p\) and \(TDS_s\) are respectively the TDS of the particle and the TDS of salt water and \(\rho_f\) is the density of fresh water. By using a buoyancy term, all drawdowns are referred to the same density, namely of fresh water. So called fresh water heads (or drawdowns in this case) are thus calculated and used in the model.

The model region (box 1) is subdivided in a number of cells. Length, height and depth of all cells is constant. At the end of every time increment \(\Delta t\), the mean concentration in every cell is calculated by averaging the concentration of all particles present in the cell. This is the concentration \(C_m^n\). If no particles are present in the cell, it means for instance that the tracer plume has already left this cell and its concentration is given the background concentration. Thereafter, dispersion is calculated with equation 4.16 but some remarks concerning the used concentration must be made. Figure 4.6 shows for a 1D case the evolution of breakthrough curves. The \(k-1\) shows the breakthrough curve due to advection and dispersion at the end of the \((k-1)\)th time step. The \(k\) shows the breakthrough curve at the \(k\)th time step due to advection. Take for instance the relative distance of 0.5. The curve at \(k-1\) shows a larger concentration gradient at this point then the curve at \(k\). Used in equation 4.16, this gradients will give different contributions due to dispersion. Therefore a weighted concentration \(C_m^w\) is defined:

\[
C_m^w = wC_m^n + (1 - w)C_m^n
\]
where \( w \) is a weighting factor commonly chosen as 0.5. So doing, the fact that dispersion takes place throughout the time increment rather than at the beginning or at the end of the advection process is taken into account. Then, the contribution of dispersion is calculated with equation 4.16. Therefore, dispersivity is constant for all layers. A longitudinal dispersivity and a horizontal and vertical dispersivity must be given. Velocities are bilinearly interpolated from the cells nodes. The concentration for cell \( m \) at the new time level \( n+1 \) is the sum of the concentration after the advection step and the concentration change due to dispersion. Next, the concentrations of all particles are updated. This is done by adding the concentration change due to dispersion in the cell where each particle is located. Finally, a new time step can start. Particles which are reaching the pumping well within 0.25 m are removed.

### 4.3.1.2 Stability criteria

Stability criteria for advective and dispersive transport are associated with the numerical scheme. If one of these criteria is not fulfilled, the time increment must be subdivided further. A first criterion is associated with advection (Konikow & Bredehoeft, 1978):

\[
\Delta t \leq \frac{\gamma L_i}{(v_i)_{\text{max}}} \tag{4.22}
\]

where \( L \) is the dimension of the cells, \((v_i)_{\text{max}}\) is the maximum seepage velocity in the \( i \)-direction (x, y or z) and \( \gamma \) is a fraction of the grid dimensions that particles will be allowed to move \((0 \leq \gamma \leq 1)\). Typically \( \gamma \) is 0.5.

Stability criterion on dispersion is based on the concentration change in a cell due to dispersion. This may not be larger than 25% of the cells initial concentration.

### 4.3.1.3 Calculation of observations

Observations during the field tests are performed with the EM39 tool, therefore output of these EM39 observations must be calculated with TRACER3D. The relative response functions shown in figure 4.2 are therefore included in the model and vertical profiles can be calculated as would be observed with the EM39. From 4.2 it can be seen that the sensitivity of the EM39 for the electrical conductivity is very small at a horizontal distance of 1.2 m from the bore hole axis and at a vertical distance of 0.3 m from the measurement point. EM39-TDS is calculated in TRACER3D by averaging the TDS of all particles within a box of 2.4*2.4*0.6 m centred around the observation point. Thereby, every particle is assigned a weight \( w_i \) based on the relative response function:

\[
w_i = \left( 1 - \left( \frac{\sqrt{16D_v^2 + D_h^2}}{1.6971} \right)^{1.5} \right)^2 \tag{4.23}
\]

where \( D_v \) is the depth difference between the particle \( i \) and the measurement centre and \( D_h \) is the horizontal distance between the particle \( i \) and the bore hole axis. The number 16 points out that particles are included in the EM39 observation torus at a four times larger horizontal than vertical distance. EM39-TDS\( j \) at the observation point \( j \) is then:
\[ EM39 - TDS_i = \frac{\sum_{i=1}^{p} W_i TDS_i}{\sum_{i=1}^{p} W_i} \] 

where TDS\(_i\) is the TDS of the \(i\)th particle and \(p\) are the number of particles used to calculated the TDS. This TDS is related with field observed electrical conductivities (our vice versa) through the formation factor. Horizontal and vertical cross-sections through the 3D weighting function to calculated EM39 observations in TRACER3D is given in figure 4.7.

![Figure 4.7](image)

**Figure 4.7** Horizontal and vertical cross-sections through the 3D weighting function to calculated EM39 observations in TRACER3D. White areas at the centre are the insensitive borehole and immediate surroundings.

### 4.3.1.4 Simulation of injection

Simulation of the injection phase and the movement of the tracer plume towards the pumping well is performed in two steps. The injection of the tracer could be simulated with the 3D model described above but this would increase computation time unnecessary. Since the injection is basically a 2D problem making abstract of the influence of lateral heterogeneities (which is moreover not included in the model), this phase is simulated with the same model presented in the above section but in 2 dimensions. The implication of this will be discussed further with the data of the field tests.

Simulation of a forced gradient tracer test is thus done in two steps:

- Injection is simulated in 2D with TRACER3D. Result is a file which gives in function of depth and distance from the well axis the concentration of the tracer around the injection well. The velocity field is calculated with HYPARIDEN according to the injection rate and time.
- This file is used as input to simulate in 3D with TRACER3D the movement of the tracer plume towards the pumping well. The tracer is considered to be distributed axial symmetrically around
the injection well at the end of the injection phase. The velocity rate is calculated with HYPARIDEN according to the discharge rate.

All boundary conditions, the parameterisation and the groundwater reservoir schematisation are the same in this two steps. Obviously, the velocity fields are different.

4.3.2 Validation of TRACER3D

Validation of HYPARIDEN can be found in Lebbe (1999a). Since this program package is the core of TRACER3D, no further validation of the computation of the drawdown calculations used in TRACER3D is needed. However, the solute transport calculation with MOC is validated with the problem of a single well tracer test. In this test, water marked with a tracer is injected in the groundwater reservoir. Breakthrough is observed in an observation well placed at a certain distance from the injection well. Flow conditions are radially diverging. The tracer concentration $C$ at a distance $r$ from the pumping well is (Gelhar & Collins, 1971):

$$C = \frac{C_0}{2} \text{erfc} \left( \frac{r^2 - r_i^2}{\left(16 \alpha L \left(\frac{r^2 - r_i^2}{3}\right)\right)^2} \right)$$

$$r_i = \sqrt{\frac{(Q/b)}{m_e}}$$

where $C_0$ is the injected tracer concentration (mg/l), $r_i$ is the average radial front position (m), $r_w$ is the well radius (m), $(Q/b)$ is the discharge per unit aquifer thickness (m²/d) and $t$ is time (d). Erfc is the complementary error function.

Simulation of a single well tracer test has been done in TRACER3D for a Theis-type of aquifer. The pumped layer has a thickness of 10 m, a hydraulic conductivity of 2 m/d and a specific elastic storage of 0.00001 m⁻¹. A tracer with a concentration of 10 g/l is injected with a discharge rate of 24 m³/d. The background concentration of the tracer is 0 g/l. Due to the radial symmetry, the problem was solved two dimensionally. The time increment is 5.76 minutes and the cell size for MOC is 0.25 m. Effective porosity is 0.38. Breakthrough curves are calculated for different values of dispersivity (0.05m and 0.1 m) and distances from the injection well and compared with the analytical solution of equation 4.25/4.26. Lateral dispersivity is 0 m.

This modelling of a single well tracer test is chosen as validation because it can be considered as a stringent test for the model. Hydraulic gradients are much larger close to the pumping well (or injection well as in this case) than at certain distance. This means that the solute transport is more difficult to be calculated more accurately. Figure 4.8 shows some of the results of the calculations. Good agreement between the numerical and analytical solution is obtained.
Figure 4.8 Comparison between simulation of a single well tracer test, calculated with TRACER3D (dots) and analytical solution by Gelhar and Collins (1971) (full line). Horizontal and vertical axis are respectively time (h) and concentration (mg/l). $D$ (m) is the distance between injection and observation well and $a$ (m) is the longitudinal dispersivity

4.4 Conformity between tracer and pumping tests

Performed on the same location and aquifer one would expect that both pumping and tracer tests will result in approximately the same values for the horizontal conductivity. With the results of both tests, breakthrough times should be predicted and/or explained coherently. Few articles dealing with combined interpretation of pumping and tracer tests are available in the hydrogeological literature. Results of those few published studies however question seriously the conformity of pumping and tracer test interpretations. Niemann & Rovey (2000) for instance find hydraulic conductivities derived from a pumping test, which are 10 to 20 times larger than derived with a tracer test. Differences are attributed to scale effects and influences of heterogeneities. Thorbjarnarson et al. (1998) on the other hand point to the difference between average aquifer horizontal conductivity derived with a pumping test and the horizontal conductivity of different layers in a aquifer derived with a tracer test. Horizons where tracer movement would be six times larger than calculated with the mean horizontal conductivity are found. Using pumping test derived average conductivities would underestimate travel distances of tracers. Mallants et al. (2000) point in this context to the importance of good estimates of conductivity in solute transport. In most studies, tracer tests are considered to be more accurate because they would implement better the heterogeneity. Freeze & Cherry (1979) have seriously questioned the uniqueness of a pumping test interpretation. They argue for ‘simpler’ well tests.

Pumping test analyses is, however, almost always done with one of the analytical interpretation methods. As has been explained in 2.6.2, stringent schematisation leads to an overestimation of the hydraulic conductivity of the pumped layer. Oversimplification of the flow towards a pumping well due to the used model and schematisation explains most, not to say all of the problems concerning the results of pumping test interpretation. The use of simpler well tests as proposed by Freeze and Cherry (1979) is thus certainly no answer to the problem. Simpler well tests use also these (in most real world cases) inadequate analytical solutions. Further, important uncertainties are introduced due to the (unknown) influences of the drilling and construction of the well. Here, we state that with proper schematisation of the groundwater reservoir and adequate tools for pumping test interpretation (as
HYPARIDEN), pumping tests and tracer tests do not provide contradictory results. This will be illustrated and discussed further in Chapter 5 with the field tests.

4.5 Derivation of Chemical Parameters

4.5.1 Push-pull test: concepts

A push-pull test is used to study in situ chemical reactions occurring in the groundwater reservoir. The method consists of the pulse-type injection (the “push”) of a test solution into the saturated zone of an aquifer through the screen of a well followed by the extraction (the “pull”) of the test solution and groundwater mixture from the same well. The test solution contains a conservative (non-reactive) tracer and one or more reactive solutes selected to investigate specific chemical and/or microbial activities. The concentrations of the reactive solutes are compared with the concentrations of the conservative tracer to deduce reaction mechanisms and rates. This test was used by Istok et al. (1997) to study microbiological activities in situ. These authors argue that the disadvantages of microcosm studies include the need for core material, the typically small and potentially unrepresentative volume of individual core samples, the potential disturbance and contamination of core material during collection, the difficulty in reproducing field conditions in an artificial laboratory environment and the potential for selective growth. Therefore, it is far better to design field tests such as the push-pull test.

A push-pull test consists of the controlled injection of a prepared test solution into a single well, followed by the extraction of the test solution and groundwater mixture from the same well. During the injection phase the test solution flows radially outward from the well casing, through the well screen and sand pack and into the saturated zone of the aquifer. The total volume $V_t (m^3)$ of aquifer investigated by the test is determined by the total injected volume $V_i (m^3)$, the volume of water stored in the well casing $V_w (m^3)$ and sand pack $V_s (m^3)$ and the effective porosity of the aquifer $n_e$ and the sand pack $n_s$:

$$V_t = \frac{V_i - V_w}{n_e} - \frac{V_s}{n_s}$$  \hspace{1cm} 4.27$$

The injected test solution penetrates an approximately cylindrical volume of aquifer centred around the well but the exact shape of this zone depends on several factors including the presence of aquifer heterogeneities, well screen length, injection rate and duration and well construction and development methods.

The composition of the test solution depends on the purpose of the test but typically consists of water containing a known concentration of a nonreactive solute and one or more reactive solutes selected to assay the activity of specific microbial enzyme system or chemical reaction. During the extraction phase flow is reversed and the test solution and groundwater mixture flows radially inward towards the well. Water samples are collected periodically during the extraction phase and the concentrations of conservative tracer, reactive solutes and any products formed by chemical reactions and/or microbial metabolism are measured and used to develop breakthrough curves for each solute. The conservative tracer breakthrough curve is used to quantify solute losses due to physical processes of advection, dispersion and diffusion. Breakthrough curves for the reactive solutes and products are used to quantify chemical and microbial activities. The breakthrough curves given in figure 4.9 illustrate this concept. A conservative tracer and a single reactive solute (the reactant) are injected. This reactant is transformed to a single product. The breakthrough curves show the relative concentration $C/C_0$ for each solute, where $C$ is the measured concentration (mg/l) and $C_0$ is the injected concentration (mg/l) versus the cumulative extracted volume when the sample was collected.
divided by the total injected volume of test solution. In this particular example the injection was followed by the injection of a small volume of solute-free water so that initial solute concentrations during the extraction phase are zero. The total quantity of each solute recovered can be obtained by integrating the area under each breakthrough curve.

![Figure 4.9](image.png)

*Figure 4.9* Single-well push-pull test: injection (upper figure) and extraction (middle figure) phase and realised breakthrough curves for the conservative tracer, reactant and formed product (lower figure) (Istok et al., 1997).

### 4.5.2 In situ determination of reaction rate coefficients

Haggerty et al. (1998) developed a simplified method of push-pull test data analyses, making possible the determination of in situ reaction rate coefficients. The goal of their work was to develop a method that (1) allows the accurate estimation of first-order reaction rate coefficients; (2) is not strongly sensitive to variations in other aquifer parameters (e.g. porosity, dispersivity); does not require the use of a numerical flow and transport code. The method is based on two simplifying assumptions: (1) the injected test solution is well mixed within the portion of the aquifer assayed by the test; and (2)
retardation factors for tracer and reactant are identical. These assumptions are identical to those commonly used in the analysis of well-mixed batch reactors.

The relative concentration (i.e., the measured concentration \(c\) divided by the injected concentration \(c_{inj}\)) of the reactant \(c_d(t)\) can be computed using (e.g., Jury & Roth, 1990):

\[
c_d(t) = c_{tr}(t)e^{-kt}
\]

where \(c_{tr}\) is the relative concentration of the conservative tracer, \(t\) is the time (h) and \(k\) is the first-order reaction rate coefficient (h\(^{-1}\)). This equation can be rewritten as:

\[
\ln\left(\frac{c_d(t)}{c_{tr}(t)}\right) = -kt
\]

So by measuring the relative concentration of the reactant and the conservative tracer and by fitting a line through a plot of \(\ln(c_d(t)/c_{tr}(t))\) versus \(t\), an estimate of the first-order reaction coefficient can be obtained.

For a push-pull test where the solution is injected as a pulse with a finite duration \(t_{inj}\), the relative concentration of the reactant at the end of the test solution’s injection is given by:

\[
c_d(t) = \frac{c_{tr}(t)\int_{0}^{t_{inj}} Q_{inj}e^{-kt} dt}{\int_{0}^{t_{inj}} Q_{inj} dt}
\]

where \(Q_{inj}\) (m\(^3\)/h) is the injection discharge rate. For a constant extraction rate \(Q\) (m\(^3\)/d) the combination of equations 4.28 and 4.30 gives:

\[
c_d(t^*) = \frac{c_{tr}(t^*)}{kt_{inj}} e^{-kt}\left(1 - e^{-k(t_{inj} + t^*)}\right)
\]

where \(t^*\) is the time elapsed since the end of the test solution’s injection. Equation 4.31 can be rewritten in a form that allows to estimate \(k\) solely from the relative concentrations of the tracer and the reactant:

\[
\ln\left(\frac{c_d(t^*)}{c_{tr}(t^*)}\right) = \ln\left(\frac{1 - e^{-kt_{inj}}}{kt_{inj}}\right) - kt^*
\]

This has the form of a simple first order equation \((y=A-kt^*)\). Thus an estimate for \(k\) can be obtained by measuring the relative concentration of conservative tracer and reactant in function of the time elapsed since the end of the injection phase using a standard least-square approach. Haggerty et al. (1998) found that the shape of the graph of \(\ln(c_d(t^*)/ c_{tr}(t^*))\) versus \(t^*\) is only very weakly dependent on variables other than \(k\).
5.1 Introduction

Three field sites were chosen to perform different parameter identification tests. The first is situated in the Belgian coastal plain near the village of Houtave. The tests are performed in Quaternary deposits. A lot of geological and hydrogeological research has been performed in the past. De Breuck et al. (1969) and Mostaert (1985) described the Quaternary deposits. Franceschi (1975) has mapped the occurrence of peat in the study area. Allemeersch (1984) studied the Holocene peat evolution. A map showing the depth of the 1500 ppm total dissolved solids (TDS) contour line was constructed by De Breuck et al. (1974) for the Belgian coastal plain and a first qualitative description of the hydrological evolution of the coastal aquifer was given (De Breuck & De Moor, 1974). De Moor & De Breuck (1969) conducted a first survey of the water quality. Recently, detailed hydrogeological studies in subregions of the coastal plain are performed as for instance by Vandenbohede (1998) and Vandenbohede & Lebbe (2002) for the area around Houtave (see also chapter 7). With this extensive background information, a first forced gradient tracer test was performed and interpreted. Main objective of the test was to collect a field data set with which TRACER3D could be tested and with which the beneficial concept of interpreting both concentration and drawdown measurements could be shown. Additionally, conclusions about aquifer hydraulic and solute transport properties and aquifer heterogeneity could be drawn. A push-pull test was also performed aiming to study aerobic respiration and denitrification in the organic material rich sediments.

As will be discussed in 5.2, the Houtave test site is only moderately heterogeneous. Therefore, a second test site with more heterogeneous sediments was selected. The Zevergem test site is situated on the heterogeneous Quaternary deposits of the Scheldt river in Belgium near the village of Zevergem. De Moor (1963) and Heyse (1979) have made sedimentological and geomorphological studies on the evolution and deposits of the Vlaamse Vallei (Flemish Valley) in which the site is situated. First hydrogeological acquaintance of the region was presented in the work of Van den Bossche (1999) who made a regional groundwater flow model. A double forced gradient tracer test, for which two injection wells and one pumping well are used, was performed. Preliminary interpretation was discussed by De Bruyne (2001). Interpretation with TRACER3D is presented here.

A third forced gradient tracer test was performed for the design of an in-situ remediation on a field site in Tessenderlo. The field site is contaminated by 1,2-dichloroethane (1,2-DCA). Its (bio)degradation in the environment is very slow (half life time of about 50 years) and it is a possible health hazard (cancerogenic). No in-situ detoxification technology with an application to groundwater is yet available. A bacteria, Desulfitobacterium dichloroeliminans strain DCA1, was identified at the
Laboratory for Microbial Ecology and Technology (LabMET) of Ghent University that can detoxify 1,2-DCA quickly in anaerobic circumstances and without producing other hazardous products (De Wildeman, 2002). To study the solute transport characteristics of the deposits in general and to aid with the design of the in-situ remediation, a forced gradient test was performed. The context of this remediation will be discussed in chapter 7 but the interpretation of the forced gradient tracer test will be shown here. This test is additionally interesting because it is performed in tertiary glauconite rich deposits.

The forced gradient tracer tests were performed on all sites in two steps. First a pumping test was done and drawdowns were measured. Then the tracer test started and concentration measurements were made. Enough time was left between pumping test and tracer test (minimum is the duration of the pumping test) so that hydraulic heads were again at their natural level.

5.2 Houtave Test Site: proof of concept

5.2.1 Introduction

The first forced gradient test was performed on a site situated in the eastern Belgian coastal plain near the village of Houtave. The field site is located east of the Stalhille Channel Ridge, an old quaternary tidal channel ridge, in the low laying polder area. Figure 5.1 shows the location of the Houtave test site. Another site, the Vijfwege test site is also indicated. Results from a previous pumping test (Vandenbohede, 1998) on this latter site are available. These can be compared with the results of the pumping test performed at the Houtave test site.

![Figure 5.1 Location of the Houtave test site and the Vijfwege test site.](image)

A hydrogeological cross-section is presented in figure 5.2. The basis of the groundwater reservoir consists of glauconite bearing clay (A) that can be treated as impermeable for this study. This is the Merelbeke Member (Gent Formation, Ieper Group) and is of early eocene age. Above it, glauconite bearing very fine sands to loamy siltous very fine sand with horizons of sandstone fragments (B) occurs. Two distinct sand stone banks are found. This is the Pittem Member also belonging to the Gent Formation, Ieper Group and can be considered a semi-permeable layer in this study. It is also of early
eocene age. Above it, grey fine sands (C) occur. The basal part of the layer contains shell fragments. This is a permeable layer and is of quaternary age. Above this permeable layer, a peat layer (D) is found. This is a paludification peat originating in a nutrient poor and water logged coversand area (Allemearsch, 1991). Organic material is also present just below the peat layer in layer C. Next, a clay layer with organic material and peat fragments (E) is found. The top layer consists of grey clay (F). The peat and clay layers are semi-permeable with the water table present in the top of the clay layer.

![Hydrogeological cross-section through the Houtave test site with the indication of screen positions.](image)

**Figure 5.2** Hydrogeological cross-section through the Houtave test site with the indication of screen positions. Numbering of layers as used in the HYPARIDEN is shown at the right hand site. A: glauconite bearing clay; B: glauconite bearing very fine sands to loamy silty very fine sand with horizons of sandstone fragments; C: grey fine sands; D: peat; E: clay layer with organic material; F: grey clay.

**Table 5.1.** Depth screen interval (m) and distance (m) from pumping well PP for the different wells used for the pumping test.

<table>
<thead>
<tr>
<th>well number</th>
<th>screen interval (mTAW)</th>
<th>distance (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PP</td>
<td>-0.80 – -5.40</td>
<td>/</td>
</tr>
<tr>
<td>PP1</td>
<td>-0.26 – -0.46</td>
<td>1.2</td>
</tr>
<tr>
<td>PP2</td>
<td>0.08 – -0.12</td>
<td>1.2</td>
</tr>
<tr>
<td>PP3</td>
<td>-7.63 – -8.63</td>
<td>2.5</td>
</tr>
<tr>
<td>PP4</td>
<td>-4.20 – -5.20</td>
<td>5.0</td>
</tr>
<tr>
<td>PP5</td>
<td>-0.60 – -1.60</td>
<td>7.3</td>
</tr>
<tr>
<td>PP6</td>
<td>-4.17 – -5.17</td>
<td>15.0</td>
</tr>
</tbody>
</table>

During the spring of 2001, fieldwork was carried out. One pumping well (PP) and six observations wells (PP1 to PP6) were installed. The rotary drill method has been applied. This means that only a

---

1 mTAW: Belgian ordnance datum TAW referring to mean low low water level, about 2.3 m below mean sea level.
very crude description of the sediments could be made. In the boreholes, PVC tubes (inner diameter of 59 mm) with screen elements were installed. Distances between observation wells and pumping well and the screen intervals are given in table 5.1.

5.2.2 (Hydro)geological site characterisation

With (hydro)geological site characterisation, derivation of geological layering and of the lateral continuity of layers is understood. This is accomplished with geophysical borehole logs. Natural gamma logs and electrical conductivity logs are used. The first log measures the natural gamma radiation of the sediments. This is mainly due to the occurrence of $^4\text{K}$, $^{238}\text{U}$ and $^{232}\text{Th}$ in clay minerals. Sediments with a large clay content will consequently have a large signal. Larger clay content means also a smaller conductivity. The natural gamma logs thus provide qualitative information about the hydraulic conductivity of the sediments. Sphere of influence is the sphere from which 90% of the measured gamma rays are coming. The radius of this sphere is between 15 to 30 cm depending on the density of the sediments, well casing and borehole or well fluids. Hence, a layer influences already the measurements although the detector is not on the same level as this layer. To measure the natural gamma of a layer without influence of surrounding layers, it must be at least as thick as the diameter of the sphere of influence. Otherwise a combination of signals from more than one layer is measured. Natural gamma radiation is measured in counts per second (cps).

![Figure 5.3 Cross-section through the Houtave test site based on natural gamma logs.](image)

Natural gamma is logged in all wells. Results of these measurements are presented in figure 5.3. The top clay and peaty clay layers are easily recognisable by their high cps. The peat layer coincides with a layer of low cps. The clay content of the peat layer is very low, hence the low counts per second. This zone thickens towards the pumping well. The contact zone between the sand and the paludification peat is heterogeneous and undulating. The permeable sand layer has an intermediate cps. Vertical as well as lateral heterogeneity is visible. The basal part of this layer has for instance a lower clay content. Note that around the level −4 mTAW, there is a zone with a lower clay content at PP6, which evolves into more clayey sediments towards the pumping well. Also in the upper part of the permeable layer, lateral heterogeneity can be observed. The deepest part of the logs show the glauconite bearing
Chapter 5: To the field

A. Vandenbohede

sandy clay to clayey sand. This unit is, however, logged in only one well, PP3 and no information of lateral heterogeneity is available.

The electrical conductivity of the sediments is measured with the EM39. Figure 5.4 shows the EM39 log in observation well PP3. A layer with high electrical conductivity is observed between 1 and 0 mTAW. This coincides with the peaty clay layer and the base of the upper clay layer. Electrical conductivity diminishes upwards because of the unsaturated zone which has a low conductivity. The peat layer has also a low electrical conductivity. The measurement of electrical conductivity does not only measure the conductivity of the sediments but also of the pore water, hence a value for the bulk electrical conductivity of the sediments is obtained. In PP3, it can be seen that below the peat layer electrical conductivity increases with depth. Here, the water becomes more saline deeper in the groundwater reservoir and the transition zone between fresh and deeper saline water is thus observed on the log. Measurements in the different wells show approximately the same profiles, hence only the data from the deepest well is presented.

![Figure 5.4 EM39-observation in PP3, before the pumping and tracer tests.](image)

A water sample was taken from PP5. With the EM39 measurements, the formation factor can be derived. The resistivity of the water sample is 3.46 $\Omega$m and the bulk conductivity at this depth is 75 mS/m, both for 11°C. After recalculating the dimensions, a formation factor of 3.85 is derived. Former measurements at the base of the pervious layer are available (Vandenbohede, 1998). The resistivity of the water is 4.13 $\Omega$m whereas the bulk resistivity is 16.00 $\Omega$m (measured with long normal configuration) resulting in a formation factor of 3.87.

5.2.3 Pumping test

The water table occurs at 1.3 m below the surface and is situated in the upper clay layer. Initially, all wells show the same potentiometric elevation coinciding with the water table. No important natural horizontal and vertical gradients occur. Further, no recharge boundaries (lakes, streams, etc.) are present in the vicinity of the site. During 24 hours, water was extracted from the pumping well with a discharge rate of 28 m$^3$/d. Drawdowns were measured with pressure probes in all observation wells. Observations are presented in figure 5.5. Just after the start of the pumping, hydraulic head was falling in wells in the pumped layer (PP4, PP5 and PP6). After 5 minutes, meaningful drawdowns were recorded in the lower semi-permeable layer (PP3). Only after 58 minutes, drawdowns were recorded in PP1, installed in the peat layer. Hydraulic head did not change measurably in PP2. All observed drawdowns are simultaneously considered during the interpretation with HYPARIDEN.
The discretisation of the groundwater reservoir in the numerical model used to simulate the pumping test is shown in figure 5.2. The lower semi-permeable layer is subdivided in three layers, layers 1, 2 and 3 respectively 7.5, 1.0 and 2.5 m thick. Layers 4, 5 and 6 represent the permeable layer and are respectively 1.0, 2.5, and 1.0 m thick. Layers 7, 8, 9 and 10 correspond with the peat layer and are respectively 0.2, 0.2, 0.1 and 0.2 m thick. Layers 11, 12 and 13 represent the peaty clay layer and are respectively 0.1, 0.2 m and 0.3 m thick. Layer 14 is the clay layer just beneath the water table and is 1.0 m thick. Discretisation of the groundwater reservoir is made in function of the lithology, where semi-permeable layers are more subdivided to simulate the predominant vertical flow, and in function of screen emplacement. Observations wells are placed in layer 2 (PP3), layer 4 (PP4 and PP6), layer 6 (PP5) and layer 8 (PP1). Drawdowns in PP2 are not considered in the interpretation because no measurable drawdowns were recorded. The screen of the pumped layer is located in the layers 4, 5 and 6. The ratio of the discharge rate in each of these layers to the total discharge rate is set equal to the ratio of the transmissivity of each of these layers to the total transmissivity of layers 4, 5 and 6.

Five different groups of parameters are deduced. The first group comprises the horizontal conductivities of layers 4, 5 and 6 along with the hydraulic resistances between them (indicated further as $K_h(4-6)$). The permeable layer is discretized in two parts, an upper (layer 6) and lower part (layer 4 and 5). Natural gamma logs in the different wells show that the upper part has a slightly larger clay content than the lower part. Initially, the ratio between the hydraulic conductivities of both parts was derived based on the drawdowns measured in the upper and lower part. This ratio $(0.72)$ was held constant for the remainder of the interpretation. Anisotropy or the ratio between horizontal and vertical conductivity was held at 5.0. The second group is the specific elastic storages of layers 4, 5 and 6 ($S_e(4-6)$). As for the conductivities, a ratio $(3.00)$ between the upper and lower part was first deduced. The third group is the horizontal conductivities of layers 1, 2 and 3 with the hydraulic resistances between them ($K_h(1-3)$). Anisotropy is also held at 5.0. The specific elastic storages of layers 1, 2 and 3 are combined in the fourth group ($S_e(1-3)$). The fifth group consists of the hydraulic resistances of layers 7, 8, 9 and 10 along with their horizontal conductivities ($c(7-10)$). Anisotropy is 132.0. The observed drawdowns are insensitive to the horizontal conductivity of the peat layer (model value is $0.15 \text{ m/d}$), the hydraulic parameters of the peaty clay layer ($K_h=0.1 \text{ m/d}$, $S_e=2.0*10^{-4} \text{ m}^{-1}$ and $K_h/K_v=5.0$), clay layer ($K_h=0.2 \text{ m/d}$, $S_e=1.0*10^{-5} \text{ m}^{-1}$ and $K_h/K_v=5.0$) and the storage coefficient near the water table $(0.04)$. These parameters are here unidentifiable and do not alter the optimal values of the derived parameter groups.

Table 5.2 Optimal parameter values derived with HYPARIDEN and their marginal $\sigma_{i}$ and conditional $\sigma_{i,j}$ standard deviation. Parameters are arranged according to sensitivity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Optimal Value</th>
<th>$\sigma_{i}$</th>
<th>$\sigma_{i,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(4-5);K_h(6)$ (m/d)</td>
<td>2.00 ; 1.44</td>
<td>0.0435</td>
<td>0.0224</td>
</tr>
<tr>
<td>$c(7-10)$ (d)</td>
<td>617.5</td>
<td>0.0328</td>
<td>0.0223</td>
</tr>
<tr>
<td>$S_e(4-5);S_e(6)$ (m$^{-1}$)</td>
<td>$0.59 10^{-4}; 0.175 10^{-3}$</td>
<td>0.0674</td>
<td>0.0223</td>
</tr>
<tr>
<td>$K_h(1-3)$ (m/d)</td>
<td>0.85</td>
<td>0.0843</td>
<td>0.0466</td>
</tr>
<tr>
<td>$S_e(1-3)$ (m$^{-1}$)</td>
<td>$0.375 10^{-3}$</td>
<td>0.1062</td>
<td>0.0717</td>
</tr>
</tbody>
</table>

Table 5.3 Partial correlation coefficients for the optimal parameter values.

<table>
<thead>
<tr>
<th></th>
<th>$K_h(4-6)$</th>
<th>$c(7-10)$</th>
<th>$S_e(4-6)$</th>
<th>$K_h(1-3)$</th>
<th>$S_e(1-3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(4-6)$</td>
<td>1.0000</td>
<td>0.6382</td>
<td>0.7293</td>
<td>-0.7140</td>
<td>-0.7553</td>
</tr>
<tr>
<td>$c(7-10)$</td>
<td>0.6382</td>
<td>1.0000</td>
<td>0.4707</td>
<td>-0.4366</td>
<td>-0.4754</td>
</tr>
<tr>
<td>$S_e(4-6)$</td>
<td>0.7293</td>
<td>0.4707</td>
<td>1.0000</td>
<td>-0.6756</td>
<td>-0.6840</td>
</tr>
<tr>
<td>$K_h(1-3)$</td>
<td>-0.7140</td>
<td>-0.4366</td>
<td>-0.6756</td>
<td>1.0000</td>
<td>0.5781</td>
</tr>
<tr>
<td>$S_e(1-3)$</td>
<td>-0.7553</td>
<td>-0.4754</td>
<td>-0.6840</td>
<td>0.5781</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Figure 5.5 shows the comparison between measured and calculated drawdowns for the layers 4, 6 and 8. Crosses are observations made during the pumping test whereas the continuous lines are the calculated drawdowns with optimal parameter values. Optimal parameter values with the marginal and conditional standard deviations are given in table 5.2. Parameters are ranked according to their sensitivity.
Figure 5.5 Comparison between the observations (crosses) and calculated drawdowns (full line) with the optimal parameters.

sensitivities. Hydraulic conductivity of the pumped layer is the most sensitive parameter and is derived with the highest accuracy. Total hydraulic resistance of the covering semi-permeable layer is the second most sensitive parameter. It is also the second most accurately derived parameter. Hydraulic conductivity grouped with the hydraulic resistance of the lower semi-permeable layer is the fourth sensitive parameter and its specific elastic storage is the least sensitive parameter. Drawdowns
measured during the beginning of the pumping in layer 2 are most sensitive to this specific elastic storage explaining why the largest deviation between observations and calculations (figure 5.5) is found here. Partial correlation coefficients are shown in table 5.3. No major correlation exists between parameters. Table 5.4 gives the condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions. Highest condition index is 5.8 indicating that only weak dependencies between parameters exist (Belsley, 1990).

With the assumption that the residuals exhibit a normal distribution as well as that the drawdowns can be approximated as a linear function within the considered region, the joint confidence region can be described by the optimal values of the parameters and the variance-covariance matrix of the parameter groups. Two-dimensional cross-sections through the joint confidence interval based on the optimal values of the parameters and the variance-covariance matrix are presented in figure 5.6. Each cross-section corresponds with a combination of two parameter groups who’s optimal values are fixed and two parameter groups who’s value change around their optimal values. Four contour lines of the sums of the squared residuals are shown. They correspond with the bounds of the 90%, 99%, 99.9% and 99.99% confidence region. Where tables 5.2, 5.3 and 5.4 describe numerically the joint confidence region of the parameters, the cross-sections give a visual representation. The graphs in the upper row

\textbf{Figure 5.6} Two-dimensional cross-sections through the 90%, 99%, 99.90% and 99.99% joint confidence interval and the best fitting normal distribution of the residuals.
of figure 5.6 show that the hydraulic conductivity of the pumped layer is derived with the largest accuracy. It can also be seen that the hydraulic resistance of the peat layer has the smallest correlation of all with the other parameters. The last graph on the first row shows that the largest correlation occurs between the specific elastic storage of the Pittem Member and the hydraulic conductivity of the pumped layer.

<table>
<thead>
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<th>Parameter η</th>
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</tr>
</tbody>
</table>

### 5.2.4 Forced Gradient Tracer Test

#### 5.2.4.1 Presentation of observations and qualitative analysis

A volume of 0.5 m³ of water with a TDS of 19 g/l was injected in PP5. After the injection of the tracer water was extracted from PP for a period of 12 days with a discharge rate of 31 m³/d. During this period the observation wells were logged daily to twice a day with the EM39 probe. Measurements in PP4 and PP3 are shown respectively in figure 5.7 and figure 5.8. After 118.6 hours, electrical conductivity between the level –1 and –2.5 rose in PP3 indicating first tracer breakthrough in the distal part from the EM39 observation torus with regard to the pumping well. The observations performed at 143.9 and 160.8 hours show a distinctive interval around –2 mTAW where the electrical conductivity is lower than above and below it. This is a small layer where hydraulic conductivity is somewhat smaller than average. Maximum tracer breakthrough occurred after approximately 184.8 hours. Afterwards electrical conductivity is decreasing. Note that in all but the last measurement, after 260.8 hours still a higher conductivity is measured around –2 mTAW whereas above and beneath this level the electrical conductivity is back to normal. This is the already mentioned horizon of smaller hydraulic conductivity in which tracer movement is a little slower.

In PP3 electrical conductivity starts to rise between the interval –1.5 to –2.5 mTAW after 184.8 hours. Maximum conductivity values are measured after about 250 hours. In comparison with PP4 the maximum electrical conductivity is less and tracer breakthrough in general is less distinct in PP3. This is due to both dispersion and advection. Due the larger travel times the tracer plume is more dispersed in PP3 then in PP4. Dispersion is the product of dispersivity and velocity. Hence, larger velocities towards the pumping well additionally enhance the dispersion. The distance dependency of the velocities (and also the time dependencies) makes that advection also accounts for the dispersion of the tracer plume. The side of the plume facing towards the pumping well moves faster then the side facing away from the pumping well. Therefore the tracer plume is thorn apart by advection. Remark that only a small sagging of the plume (less than 0.20 m) can be observed. The horizontal movement of the tracer plume due to the pumping is by far more important than density effects.

Besides the tracer movement the conductivity measurements also show upconing of the fresh-salt water transition zone. Only PP3, which is the observation well closest to the pumping well, provides observations under the level of the pumping well and is therefore optimally placed to measure this upconing. Figure 5.9 shows the evolution of TDS with time in the well PP3 for the depth interval below the tracer plume. Most of the upconing happens in the first six to seven days. Thereafter, the transition zone does not move much further upwards. Below the level –7 mTAW, upconing becomes
very small due to the low vertical velocities. The 9000 mg/l isoconcentration line undergoes the maximum vertical upward movement. This line is initially 0.5 m beneath the bottom of the pumping
well. In the upper part of the pumped layer movement of isoconcentration lines is small due to the dominant horizontal velocity towards the pumping well.

Figure 5.9 TDS-evolution in function of depth and time for PP3. Upconing of the isoconcentration lines between 5000 and 14000 mg/l in PP3 is shown on the right

With the EM39 probe a measurement has been done every 20 cm. This means that tracer breakthrough curves can be studied on different levels in the observation wells. This is presented here by the relative times of maximum breakthrough. For every level in which the tracer moves the time of maximum concentration $T_i$ is determined and the mean time $T$ is calculated from $n$ $T_i$:

$$T = \frac{\sum_{i=1}^{n} T_i}{n}$$

Figure 5.10 shows the ratio $T/T_i$ for the different levels in PP4 and PP3. If $T/T_i$ is larger than 1, than the time of tracer breakthrough is less than average and the horizontal conductivity is larger than average. If $T/T_i$ is less than 1, than the time of tracer breakthrough is larger than average and the horizontal conductivity is less than average. Therefore with such profiles vertical heterogeneity can be studied and individual layers can be identified within an apparent homogeneous unit. If these layers are lateral homogeneous the same profiles should be derived in different observation wells. This is the case below the level of –2.3 mTAW. At –2.7 mTAW a horizon with a slightly smaller conductivity can be seen. Above –2.3 mTAW the velocity profiles in PP3 and PP4 are not completely the same.

Figure 5.10 Relative time of maximum tracer breakthrough in function of depth for PP4 and PP3.
This is due to lateral heterogeneity. In PP4 a zone with lower conductivity is observed around –2.1 mTAW. This coincides with a more clayey lens observed only in PP4 with the gamma log. Above this level a layer with higher hydraulic conductivity exists. This is found on a slightly higher level in PP3. In general, from this velocity profiles it can be learned that just below the peat layer a lateral heterogeneous layer exist. This layer is probably a heterogeneous transition zone between the permeable sand layer and the less permeable peat layer that was also suggested on basis of the gamma logs. Below this zone the vertical heterogeneity is far more important then lateral heterogeneity. T/T is limited between 0.95 and 1.1. This shows that the range of hydraulic conductivity occurring in the upper part of the permeable sand layer is limited.

5.2.4.2 Interpretation with an analytical model

Breakthrough curves presented in figures 5.7 and 5.8 are first analysed with an analytical formula. This was done to see in a quick and simple way if the tracer test and pumping test data give approximately the same result. This was done to prove our point that when a pumping test is interpreted correctly, pumping test interpretation and tracer test interpretation should lead to similar results. This was questioned by Niemann & Rovey (2000) using a Theis interpreted pumping test. Movement of tracer in the groundwater reservoir is governed by the advective-dispersive equation. First the injected water forms a cylinder around the injection well. Injection volume and porosity determine the cylinder radius. It is further assumed that density effects on the time of maximum tracer breakthrough in the two observation wells are negligible small. This can be stated because of the nature of the tracer tests and is confirmed by the description of the upconing and by the near equal level of maximum tracer breakthrough in PP4 and PP3. It is a forced tracer test by which the injected volume of water is pulled mainly horizontally towards the pumping well. The horizontal flow component towards the pumped well is much larger than the vertical downward component due to density differences between fresh and salt water. With this considerations the three dimensional advective-dispersive equation is solved analytical for a tracer moving along a streamline between injection point and pumping well (after Moltyaner, 1987):

\[
C(x, y, t) = \frac{C_0}{4} \left( \text{erf} \left( \frac{x + r/2 - v \cdot t}{2\sqrt{D_L t}} \right) - \text{erf} \left( \frac{x - r/2 - v \cdot t}{2\sqrt{D_L t}} \right) \right) \left( \text{erf} \left( \frac{y + r/2}{2\sqrt{D_T t}} \right) - \text{erf} \left( \frac{y - r/2}{2\sqrt{D_T t}} \right) \right)
\]

where \( C \) is tracer concentration (mg/l); \( C_0 \) is concentration of the injection water (mg/l); \( D_L \) and \( D_T \) are respectively longitudinal and transverse dispersion (m²/d); \( x \) and \( y \) are cartesian co-ordinates (m) with the \( x \)-axis along the mean flow direction; \( r \) is the radius of the initial cylinder of injection water (m); \( v \) is the constant seepage velocity (m/d) between injection point and observation point and \( t \) is time (d). Erf is the error function. The horizontal \( x \)-\( y \) plane in which tracer movement occurs goes through the half depth of the injection well. Longitudinal and transverse dispersions are given by:

\[
D_L = \alpha_L v \\
D_T = \alpha_T v
\]

\( \alpha_L \) and \( \alpha_T \) are respectively longitudinal and transverse dispersivity (m). Despite the longitudinal and transverse dispersion and the groundwater flow velocity, all parameters in equation 5.2 are known. During a forced gradient test the groundwater velocity is time and distance dependent. However, between the injection and observation well a mean velocity can be determined. The time of maximum breakthrough concentration on the observation points is only depended on this mean velocity. This mean velocity can be deduced in two different ways. It can be deduced starting with the concentration measurements during the tracer test using equation 5.2 or with the head measurements and the results
of the pumping test. Both results should be in close agreement with each other assuming that tracer and pumping test analysis will lead to more or less to the same results.

With equation 5.2 concentration changes in time are calculated for PP4 and PP3. These calculations are shown in figure 5.11 (full line) for the observation wells. For every observation time, concentrations are calculated in function of distance from the injection well. With these, the concentrations which should be measured with the EM39 probe are calculated. Therefore, concentrations are weighted in function of distance from the EM39 (McNeill et al. 1990; see figure 4.1). These are then compared with the breakthrough curve on the level on which tracer concentrations are largest. Three unknown parameters are present in equation 5.2, the mean seepage velocity between injection well and observation point and the longitudinal and transverse dispersion. The former is determining the time of maximum tracer breakthrough, the latter two the concentration spread around the mean. By trial and error the calculated curve and the observations were fitted. Mean groundwater velocity of 0.30 m/d between injection well and PP4 and 0.48 m/d between injection well and PP3 are derived.

Figure 5.11 Fit between the observations and analytical model for the observations in PP4 (A) and PP3 (B).

Velocity at a certain observation point inside the influence radius is time and distance dependent during the course of a pumping test. Mean seepage velocity $v$ between injection and observation well at a certain time $t$ after the start of pumping is:
5.4

\[ v = K_h \frac{I}{n_e} \]

\( K_h \) is the horizontal conductivity (m/d) of the layer in which the tracer moves, \( I \) the mean hydraulic gradient (-) between injection well and observation well and \( n_e \) is the effective porosity (-). Hydraulic gradients can be considered in \( k \) equal steps between injection and observation well. Mean seepage velocity between the injection and observation well is then:

\[ v = \frac{K_h}{k \cdot n_e} \sum_{i=1}^{k} I_i \]

5.5

If this gradient is considered to be constant during a time \( \Delta t \) (d), the mean seepage velocity between injection and observation well from start of the pumping until a time \( T \) (d) is:

\[ v = \left( \frac{1}{T} \sum_{i} \left( \frac{K_h}{k \cdot n_e} \sum_{i=1}^{k} I_i \Delta t \right) \right) \]

5.6

Different points (\( k \)) between injection and observation well are considered in equation 5.6 to improve accuracy.

These mean seepage velocities are calculated between the injection well and observation wells PP4 and PP3 based on the results of the pumping test interpretation. With a schematisation of the groundwater reservoir and values for the different hydraulic parameters, a pumping test can be simulated with the axial-symmetric numerical model of the HYPARIDEN program package. During the tracer test, salt water was injected in layer 6 of the numerical model. The pumping during the tracer test is modelled according to the optimal hydraulic parameters as derived from the pumping test and with the same reservoir schematisation. Drawdowns are calculated in layer 6 at distances of 2.5, 3.8, 5.0, 6.2, and 7.3 m from the pumping well. Thereafter, mean seepage velocities between the injection well and observation wells PP4 and PP3 are calculated as shown in equation 5.6. The mean seepage velocity between injection and observation well PP4 is thereby 0.30 m/d and the mean velocity between injection and observation well PP3 is 0.47 m/d. This is calculated with a porosity of 0.40. By using the inverse numerical model, mean seepage velocities are calculated based on realistic reservoir schematisation and incorporating the leakage from semi-permeable layers. These mean seepage velocities fit very well the mean seepage velocities derived from the tracer test data. This means that the time of maximum breakthrough can be predicted with hydraulic parameters inferred from the pumping test. So, the drawdown and concentration data lead in this case to the same result.

A porosity of 0.40 is used here. Porosity values derived by means of the grain size analyses (Franceschi, 1975) and based on the Scherer (1987) (see section 3.3.2) relationship range between 0.36 and 0.41 with a mean value of 0.385 and a standard deviation of 0.02.

5.2.4.3 Analytical pumping test interpretations

The pumping test was analysed using the analytical models of Theis, Jacob-Hantush, Hantush and Boulton-Cooley to see the difference in inferred hydraulic conductivity values using these models. Thereafter with HYPARIDEN and the derived value for the hydraulic conductivity mean seepage velocities are calculated as described in 5.2.4.2. Hydraulic conductivities and mean velocities are presented in table 5.5.
Mean seepage velocities are calculated with a porosity of 0.4. All conductivity values inferred from the analytical models are too large as explained in 4.2.1. The leakage is ignored or severely underestimated in all these methods. The calculated mean groundwater flow velocities are thus also too large. With equation 5.2 tracer breakthrough curves are calculated for observation wells PP4 and PP3 (figure 5.12). It is obvious that with the analytically derived conductivities the breakthrough curves can not be reconstructed unless unrealistically high values for porosities are used: 2.1 for the method of Theis, 1.3 for the method of Jacob-Hantush, 1.0 for the method of Hantush and 1.7 for the method of Boulton-Cooley. Remark also that the model of Theis that neglects completely inflow from surrounding semi-permeable layers has the greatest deviation from the observations. This is partly solved in the other analytical formulations but strict boundary conditions prevent prediction of maximum tracer breakthrough in the observation wells.

**Table 5.5** Horizontal hydraulic conductivity $K_h$ (m/d), mean seepage velocity between injection point and observation well PP4 $v_{PP4}$ (m/d) and mean seepage velocity between injection point and observation well PP3 $v_{PP3}$ (m/d) for pumping test analyses with different models.

<table>
<thead>
<tr>
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<th>$K_h$ (m/d)</th>
<th>$v_{PP4}$ (m/d)</th>
<th>$v_{PP3}$ (m/d)</th>
</tr>
</thead>
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<tr>
<td>Invers Numerisch model</td>
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<td>0.30</td>
<td>0.47</td>
</tr>
<tr>
<td>Theis</td>
<td>6.98</td>
<td>1.59</td>
<td>2.44</td>
</tr>
<tr>
<td>Jacob-Hantush</td>
<td>4.14</td>
<td>0.94</td>
<td>1.45</td>
</tr>
<tr>
<td>Hantush</td>
<td>3.30</td>
<td>0.75</td>
<td>1.15</td>
</tr>
<tr>
<td>Boulton-Cooley</td>
<td>4.86</td>
<td>1.11</td>
<td>1.70</td>
</tr>
</tbody>
</table>

**Figure 5.12** Different breakthrough curves for PP4 (A) and PP3 (B). The mean seepage velocities are calculated with the pumping test interpretation of Theis (1), Jacob-Hantush (2), Hantush (3), Boulton Cooley (4) and HYPARIDEN (5).

5.2.4.4 Dispersivity values from the tracer test

From the tracer test data and equation 5.2, a value for longitudinal and transverse dispersion can be derived (table 5.6). With the mean seepage velocities the longitudinal dispersivity can be found by matching the calculated and observed concentrations by trial and error. The ratio between longitudinal and transverse dispersion is set at 10. Longitudinal dispersivities are larger for PP3 than for PP4. Transverse dispersion is relatively large. This is however an artefact of the tracer test layout. The velocity field is time and distance depended. This means that the side of the salt water body facing the pumped well experiences always a greater velocity then the side facing the injection well due to the different distances from the pumped well. Every point in the tracer body undergoes thus at a certain
time a different velocity. Basically the tracer body is torn apart by this velocity field. The difference grows as the tracer moves towards the pumping well because gradients are larger and the tracer body is more dispersed. In equation 5.2 constant mean seepage velocities between injection and observation well are used which do not model the dispersion of the tracer body by the velocity field. This result in the observed upscaling of the longitudinal dispersivity both needed to explain the breaking up of the tracer body in the modelled velocity field. Significance of the dispersivities shown in table 5.6 is thus very restricted.

Table 5.6 Longitudinal and transverse dispersivity (m) derived from PP4 and PP3.

<table>
<thead>
<tr>
<th></th>
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<tr>
<td>(\alpha_L)</td>
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<tr>
<td>(\alpha_T)</td>
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5.2.5 3D simulation with TRACER3D

The discretisation of the groundwater reservoir used for interpretation of the pumping tests is used as basis for the discretisation of the groundwater reservoir in TRACER3D. The lower semi-pervious and pervious layer are further divided in smaller model layers to enhance accuracy of the model. Basis of the groundwater reservoir is the clay of the Merelbeke Member which is considered impermeable in this study. The very fine sands to loamy siltous very fine sand of the Pittem Member is divided in 5 layers of respectively 7.5, 1, 1, 1 and 0.5 m thick. The quaternary pervious layer is divided from bottom to top in 4 layers of respectively 0.5, 0.5, 0.4, 0.3 and 14 layers of 0.2 m thickness. The discretisation of the top peat and clay layers remains unchanged. The model is therefore run with 31 model layers. The hydraulic parameters derived with the pumping test are used after recalculation of the hydraulic resistance to the new layer thickness with a conductivity anisotropy of 5. A transition zone (layer 14 to 16) is modelled between the upper and lower part of the pervious layer. No sharp boundary is visible on the natural gamma logs between these parts. In the discretisation of the pumping test, this boundary must be sharp due to modelling purposes but is of importance for the modelling of solute transport.

With this discretisation the injection of the tracer is first simulated. The TDS of the groundwater increases deeper in the groundwater reservoir, see the EM39 profile of PP3 (figure 5.4). These observations of the background TDS were brought into the model with concentration layers of 0.5 m thickness. As explained in chapter 4, injection is modelled two-dimensionally. The cross-section is 6 m high and has a width of 4 m. The injection well is placed centrally and the top is at 1 m TAW. Hence, only the area which is of importance during the injection of the tracer is modelled. In the solute transport box particles with a in-between distance (horizontal and vertical) of 5 cm are defined. In this way, the model starts with 29049 particles. For every particle, an initial TDS is calculated with interpolation of its vertical position with regard to the position of the concentration layers. During 3.5 hours the tracer is injected at a rate of 3.223 m³/d or 0.47 m³ of tracer is injected. The filter of the injection well is installed in the top of the pervious layer. During the modelling of the forced gradient test, it became clear that the tracer not only had entered the groundwater reservoir on the level of the screen interval but also on deeper levels. So, during the interpretation of the tracer test, the calculated distribution of the tracer around the injection well was corrected. The reasoning behind this is further explained and illustrated in section 5.5. The period of 3.5 hours was divided in 300 timesteps. This relatively large amount of steps was needed to fulfil the stability criteria which are built into the model. During every time step 160 particles are injected in the groundwater reservoir.
Figure 5.13 Comparison of observations (dots) and calculations (full line) for PP4 modelling only advective transport. Horizontal axis is TDS (mg/l) and vertical axis is the level (mTAW).
The same discretisation of the groundwater reservoir is used to model the forced gradient test. The model area has a surface of 11.5 x 3.0 m². In this modelling box (box 1) particles are placed with an in-between distance of 10 cm. In a second box (box 2) with a height of 6 m, length of 6.5 m and width of 3 m the particles are placed with an in-between distance of 5 cm. This last box is centred around the injection well. The same concentration layers are defined and a concentration is calculated for every particle. All 18 layers in which the pervious layer is subdivided are pumped with a discharge rate of 31 m³/d. The model is run over 400 hours in 40 time steps. This time discretisation is sufficient to fulfil the stability criteria. 296033 particles are used in the model. Observations are calculated on the position of observation well PP4 and PP3. In different runs the porosity and dispersivity were determined. As mentioned before, the initial concentration distribution around the injection well had to be slightly changed.

Comparison between observations in PP4 and the calculations is shown in figure 5.13. For this calculation only advective transport is considered. With even a small dispersivity of 1 mm the maximum concentration of breakthrough is calculated to low. Figure 5.14 shows the comparison of observed and calculated breakthrough curves on the level of maximum tracer breakthrough in PP3 and PP4. The porosity which is used is 0.39.

Figures 5.13 and 5.14 show that the time of maximum tracer breakthrough can be modelled accurately and that a good fit between observed and calculated concentrations in PP4 was achieved. Comparison between observations and calculations shows further that with TRACER3D tracer breakthrough curves can be modelled. Only during the first part of the tracer breakthrough the fit is not very good. For the observations of 118.6 and 143.9 hours after start of the pumping, calculated concentrations are too high in the lower part of the tracer plume. This is probably due to local small heterogeneities which deviate the true from the calculated velocity field. With only advective transport it is clear from figure 5.14 that the breakthrough curve of PP3 can not be modelled at all. The maximum concentration is too large and tracer breakthrough starts too late. This means that the tracer is not dispersed enough. Note that the time of maximum tracer breakthrough however is approximately right. To model tracer breakthrough of PP3 more accurately both advective and dispersive transport must be considered. Figure 5.15 shows the comparison between observed (dots) and calculated (full line) TDS taking into account advective and dispersive transport. Best fit between observations and calculations in PP3 was accomplished with a longitudinal dispersivity of 0.1 m. Ratio between longitudinal and transverse dispersivity is set at 10. All other parameters are the same. With a longitudinal dispersivity of 0.1 m the calculated breakthrough curve for PP4 obviously does not fit the observations (figure 5.16). The maximum concentration is too low. Note that there is also a small shift in the time of maximum concentration breakthrough.
Figure 5.15 Comparison between observed (dots) and calculated (full line) TDS for PP3.

Figure 5.16 Comparison between observations (dots) and calculations (full line) on the level of maximum tracer breakthrough in PP4 and PP3, simulating advective and dispersive transport.
Figure 5.17: Comparison between the hydraulic conductivity values derived from the pumping and recovery tests and the forced gradient test.

Figure 5.17 shows the comparison of the horizontal hydraulic conductivity derived with the pumping test and with the tracer test. Only small differences exist. The boundary between the upper and lower part of the pumped layer is sharp in the pumping test analyses due to the discretisation which is dependent on both the lithology and screen placement. This boundary could be modelled in more detail during the tracer test interpretation. It turned out not to be a sharp boundary. Instead a transition zone between the two is determined as can be seen on the gamma log data.

5.2.6 Sensitivity analyses

Sensitivity analyses provide a very useful tool to deduce which parameters can be derived with a certain test and what their reliability is. This is used here to show the benefits of a forced gradient tracer test (interpretation of drawdown and concentration data) over a pumping test (interpretation of only drawdown data) and a tracer test (interpretation of only concentration data). With the sensitivity analyses it is further shown that the use of both drawdown and concentration measurements enhance the reliability of the derived solute transport and hydraulic parameters. For the sensitivity analyses presented here concentration observation at PP3 and PP4 and drawdown observations in PP4, PP5 and PP6 are calculated and the sensitivities of hydraulic and solute transport parameters of the permeable layer are derived. The parameter values derived in section 5.2.5 on forced gradient test are used. Longitudinal $\alpha_L$ and transverse dispersivity $\alpha_T$ are respectively 0.05 m and 0.005 m. This is half the value derived with concentration observations in PP3. Recall that in the sensitivity analyses a parameter is changed by a factor, the sensitivity factor $sf$, and the output of the model is compared with the output calculated before the change. A parameter is sensitive if this output changes considerably. The sensitivity of the $i^{th}$ observation for $j^{th}$ parameter is:

$$J_j = \frac{\log_{10} s_i(p^*_if) - \log_{10} s_i}{\log_{10} sf}$$

where $s_i$ is the calculated drawdown or concentration corresponding with the $i^{th}$ observation using the initial parameters, $s_i(p^*_if)$ is the calculated drawdown or concentration corresponding with the $i^{th}$ observation using the initial parameters except the $j^{th}$ parameter which is multiplied by the sensitivity factor. Two different values for the sensitivity factor are used. The sensitivity factor used to calculated drawdown sensitivities and concentration sensitivities for porosity is $10^{0.1}$. For the other concentration sensitivities the sensitivity factor is $10^{0.3}$, this to cause larger changes.
Figure 5.18 shows the drawdown sensitivities of the hydraulic conductivity, hydraulic resistance and specific elastic storage for the observations in wells PP4, PP5 and PP6. Horizontal conductivity is the most sensitive parameter with respect to drawdown observations followed by specific elastic storage and hydraulic resistance. The drawdown sensitivities for the hydraulic resistance are positive for small values of $t/r^2$ (in which $t$ is time and $r$ is the distance from the pumping well) and negative for large values of $t/r^2$ as described by Lebbe (1988). Sensitivities evolve towards a constant value. These values are function of the distance from the pumping well. The well closest towards the pumping well (PP4) has the largest negative drawdown sensitivities after long pumping time. Wells placed farther away from the pumping well evolve to smaller negative sensitivities. Drawdown sensitivities for the specific elastic storage are negative. Right after the start of the pumping, sensitivities are largest and they diminish with time. Sensitivities become zero when the groundwater flow has reached equilibrium. Sensitivities are smallest for the well closest to the pumping well. Drawdown sensitivity of hydraulic resistance of the pervious layer can be positive as negative. Sensitivities for PP4 and PP6, both in the lower part of the pervious layer, show the same trends. Sensitivities for PP5, placed in the upper part of the layer, show also the same trend but with opposed sign.

Table 5.7 Partial correlation coefficients and marginal and conditional standard deviation due to drawdown observations.

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<tr>
<td>$c$</td>
<td></td>
<td></td>
<td>1.0000</td>
<td>0.0019</td>
<td>0.0002</td>
</tr>
</tbody>
</table>

Table 5.7 gives the partial correlation coefficients and marginal and conditional standard deviation for the three parameters. Parameters are arranged according to sensitivity. The largest correlation is found between conductivity and specific elastic storage. From the marginal and conditional standard
deviations it can be concluded that the conductivity and the specific elastic storage can be determined with the largest accuracy. Vertical conductivity can also be derived but with a smaller accuracy.

Table 5.8 gives the condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions due to the drawdown observations. Dependencies between parameters are weak. The largest condition index is only 9.0860. This axis of the joint confidence interval influences only the marginal variance of the hydraulic resistance considerably (for 99.98%).

![Figure 5.19](image_url)

**Figure 5.19** Concentration sensitivities for effective porosity and hydraulic resistance in observation wells PP3 and PP4 for the depth interval of tracer breakthrough. Horizontal axis is time since the start of the test (days) and vertical axis is depths (mTAW). Colour scale for the sensitivities is on the right-hand side of each figure.
Figure 5.20 Concentration sensitivities for horizontal hydraulic conductivity and longitudinal dispersivity in observation wells PP3 and PP4 for the depth interval of tracer breakthrough. Horizontal axis is times since the start of the test (days) and vertical axis is depths (mTAW). Colour scale for the sensitivities is on the right-hand side of each figure.

Table 5.8 Condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions due to the drawdown observations.

<table>
<thead>
<tr>
<th>$\eta$ parameter</th>
<th>$\mu$</th>
<th>$\pi_1$</th>
<th>$\pi_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h$</td>
<td>0.5941</td>
<td>0.3655</td>
<td>0.0404</td>
</tr>
<tr>
<td>$S_s$</td>
<td>0.0472</td>
<td>0.8560</td>
<td>0.0968</td>
</tr>
<tr>
<td>$C$</td>
<td>0.0000</td>
<td>0.0002</td>
<td>0.9998</td>
</tr>
</tbody>
</table>

Concentration sensitivities of all parameters ($K_h$, $S_s$, $c$, $n$, $\alpha_L$ and $\alpha_T$) for observations with the EM39 tool in observation wells PP3 and PP4 are calculated for the interval of tracer breakthrough. Effective porosity is the most sensitive parameter followed by hydraulic resistance, horizontal conductivity, longitudinal dispersivity, transverse dispersivity and specific elastic storage. From these sensitivity analyses it follows that the parameters determining advective transport are more sensitive than the
parameters describing dispersion. This is due to the small dispersivity values. Advective transport is the dominating process. Figure 5.19 show the concentration sensitivity for the effective porosity and hydraulic resistance in observation wells PP3 and PP4. Due to a larger effective porosity, the velocities are smaller and tracer breakthrough occurs later. Sensitivities are therefor first negative and turn to positive after tracer breakthrough. Concentration sensitivities for the hydraulic resistance are positive. This means that tracer breakthrough occurs later. Due to the larger hydraulic resistance between layers leakage between layers is smaller and horizontal flow is smaller. Figure 5.20 shows the concentration sensitivity for the horizontal hydraulic conductivity and longitudinal dispersivity in observation wells PP3 and PP4. Concentration sensitivities for the hydraulic conductivity are complex. They are positive in the upper part of the tracer plume and negative in the lower part. This means that by enlarging the hydraulic conductivity of the pervious layer the tracer moves slower in the upper part and quicker in the lower part. The concentration sensitivities of the longitudinal dispersivity can be negative or positive. With a larger dispersivity the tracer is more dispersed. The maximum concentration during breakthrough is lower, hence the central negative sensitivities. The tails are however longer hence the positive sensitivity. Sensitivity of concentration observations to the transverse dispersivity is not given because these parameters are almost insensitive.

Table 5.9 gives the partial correlation coefficients and the marginal and conditional standard deviation for the six parameters. Partial correlation coefficients point out only weak correlation between parameters. The largest correlation is found between the longitudinal dispersivity and effective porosity. Effective porosity is the parameter which can be derived most accurately from this data set. Hydraulic resistance, horizontal conductivity and longitudinal dispersivity can also be derived. Transverse dispersivity and specific elastic storage however can not be found. Two condition indices (35.69 and 68.59) point to strong dependencies. These condition indices define almost completely the marginal variance of the transverse dispersivity and the specific elastic storage (table 5.10).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>n_e</th>
<th>c</th>
<th>K_h</th>
<th>α_L</th>
<th>α_T</th>
<th>S_s</th>
<th>s_mj</th>
<th>s_cj</th>
</tr>
</thead>
<tbody>
<tr>
<td>n_e</td>
<td>1.0000</td>
<td>-0.0958</td>
<td>0.4664</td>
<td>-0.5166</td>
<td>0.1168</td>
<td>0.0510</td>
<td>0.0003</td>
<td>0.0009</td>
</tr>
<tr>
<td>c</td>
<td>1.0000</td>
<td>-0.2980</td>
<td>0.0393</td>
<td>0.8067</td>
<td>-0.1461</td>
<td>0.0010</td>
<td>0.0004</td>
<td></td>
</tr>
<tr>
<td>K_h</td>
<td>1.0000</td>
<td>-0.1523</td>
<td>-0.4530</td>
<td>0.2644</td>
<td>0.0014</td>
<td>0.0011</td>
<td></td>
<td></td>
</tr>
<tr>
<td>α_L</td>
<td>1.0000</td>
<td>-0.4780</td>
<td>0.2080</td>
<td>0.0033</td>
<td>0.0027</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>α_T</td>
<td>1.0000</td>
<td>-0.5034</td>
<td>0.0882</td>
<td>0.0041</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S_s</td>
<td>1.0000</td>
<td>0.0117</td>
<td>0.0111</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.10 Condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions due to the concentration observations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>n_e</th>
<th>c</th>
<th>K_h</th>
<th>α_L</th>
<th>α_T</th>
<th>S_s</th>
</tr>
</thead>
<tbody>
<tr>
<td>n_e</td>
<td>0.5397</td>
<td>0.0567</td>
<td>0.0681</td>
<td>0.2896</td>
<td>0.0460</td>
<td>0.0000</td>
</tr>
<tr>
<td>c</td>
<td>0.0000</td>
<td>0.5557</td>
<td>0.3879</td>
<td>0.0345</td>
<td>0.0012</td>
<td>0.0208</td>
</tr>
<tr>
<td>K_h</td>
<td>0.0000</td>
<td>0.1101</td>
<td>0.4296</td>
<td>0.02736</td>
<td>0.0655</td>
<td>0.1210</td>
</tr>
<tr>
<td>α_L</td>
<td>0.0000</td>
<td>0.0004</td>
<td>0.0060</td>
<td>0.6943</td>
<td>0.1911</td>
<td>0.1082</td>
</tr>
<tr>
<td>α_T</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0002</td>
<td>0.0052</td>
<td>0.4869</td>
<td>0.5076</td>
</tr>
<tr>
<td>S_s</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0692</td>
<td>0.9308</td>
</tr>
</tbody>
</table>

When observations of concentration and drawdowns are analysed simultaneously more parameters can be derived than is the case when only one set of data is used. Accuracy of derived parameters is also higher. Table 5.11 shows the partial correlation coefficients and the marginal and conditional standard deviation due to drawdown and concentration observations. Table 5.12 gives the condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions both due to the drawdown and concentration observations together. Effective porosity is still the most sensitive parameter but followed now by horizontal conductivity, specific elastic storage, hydraulic resistance, longitudinal
and transverse dispersivity. The parameters describing advective transport are again more sensitive than the dispersivities. The most obvious change in comparison with sensitivities using only concentration observations is the specific elastic storage. This parameter is very sensitive during the first part of the test to drawdown measurements. High drawdown sensitivity of the conductivity makes it the second most sensitive parameter. Partial correlations are again very small, the largest occurring between the longitudinal dispersivity and porosity. Only one condition index points to a strong dependency. The others show weak to very moderate dependencies. The condition index of 36.8 defines for 98.81% the marginal variance of the transverse dispersivity. This parameter can therefore not be derived by the used observations. The marginal variance of the longitudinal dispersivity is defined by 44.96% by the largest condition index and can be determined the least accurately.

Table 5.11 Partial correlation coefficients and the marginal and conditional standard deviation for the drawdown and concentration observation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>n</th>
<th>Kh</th>
<th>Ss</th>
<th>c</th>
<th>α_L</th>
<th>α_T</th>
<th>s_m</th>
<th>s_c</th>
</tr>
</thead>
<tbody>
<tr>
<td>N_e</td>
<td>1.0000</td>
<td>0.1128</td>
<td>0.0425</td>
<td>0.0277</td>
<td>-0.5122</td>
<td>0.4115</td>
<td>0.0001</td>
<td>0.0001</td>
</tr>
<tr>
<td>K_h</td>
<td>0.0000</td>
<td>1.0000</td>
<td>0.4267</td>
<td>-0.1297</td>
<td>-0.0462</td>
<td>-0.0939</td>
<td>0.0001</td>
<td>0.0001</td>
</tr>
<tr>
<td>S_s</td>
<td>1.0000</td>
<td>-0.1409</td>
<td>0.0000</td>
<td>0.0663</td>
<td>-0.0752</td>
<td>0.0003</td>
<td>0.0001</td>
<td>0.0016</td>
</tr>
<tr>
<td>c</td>
<td>1.0000</td>
<td>-0.1409</td>
<td>0.0000</td>
<td>0.0663</td>
<td>-0.0752</td>
<td>0.0003</td>
<td>0.0001</td>
<td>0.0016</td>
</tr>
<tr>
<td>α_L</td>
<td>1.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>α_T</td>
<td>1.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Table 5.12 Condition indexes µ and π matrix of marginal variance-decomposition proportions due to the drawdown and concentration observations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>µ</th>
<th>π</th>
</tr>
</thead>
<tbody>
<tr>
<td>n_e</td>
<td>0.6561</td>
<td>1.3372</td>
</tr>
<tr>
<td>K_h</td>
<td>0.0165</td>
<td>0.6035</td>
</tr>
<tr>
<td>S_s</td>
<td>0.0002</td>
<td>0.0437</td>
</tr>
<tr>
<td>c</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>α_L</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>α_T</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

5.2.7 Identification of transverse dispersivity

Relatively few field values of transverse dispersivities are reported from field tests. Sudicky & Cherry (1979), Sudicky et al. (1983) and Moltyaner & Killey (1988) for instance provide values derived from natural-gradient tests. Gelhar et al (1992) gives an overview of the available literature and discusses the ratio of longitudinal to transverse dispersivity. Interpretations methods are readily available, reliable derived values are harder to find. Zou et al. (1994) presents, for instance, a two-dimensional model to estimate longitudinal and transversal dispersions in an uniform groundwater flow field after slug tracer injection. Recently, Chen et al. (1999) developed a two-dimensional model estimating the effects of longitudinal and transverse dispersivity simultaneously in a radially convergent flow field.

Observation wells placed laterally of the line injection well – pumping well are use to get a three-dimensional view of a tracer plume. It is further expected that these observation wells will be more sensitive to transverse dispersion than a centrally placed well. The possibility of determining transverse dispersivity with a laterally placed well is investigated through the diagnostics of the sensitivity analyses. In the same way as described in section 5.2.6 the concentration sensitivities are calculated for PP3, PP4 and PP7. PP7 is a fictitious well placed centrally between PP3 and PP4 but of line by 0.75 m. Condition indexes µ and π matrix of marginal variance-decomposition proportions due to the concentration observations are shown in table 5.13. Despite the additional information of a
lateral observation well the same conclusion can be drawn as in section 5.2.6. Two condition indices indicate strong dependencies between parameters. These two define respectively for 57.09% (for CI=39.0327) and 42.58% (for CI=71.0406) the marginal variance of the transverse dispersivity.

Other positions of PP7 have also been considered. PP7 has been set 0.5 an 1.0 m lateral of the line injection well and pumping well but the diagnostics remain the same. With a forced gradient test and the kind of observations used here transverse dispersivity can not be identified. The reason is of course the very small value (0.005 m). Given a ratio between longitudinal and transverse dispersivity of 10 in most cases (Gelhar et al, 1992), the identification in general of transverse dispersivity with a forced gradient test is questionable.

Table 5.13 Condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions due to the concentration observations in PP3, PP4 and a fictitious PP7.

<table>
<thead>
<tr>
<th>$\eta$ parameter</th>
<th>1.0000</th>
<th>4.8377</th>
<th>5.9046</th>
<th>15.3766</th>
<th>39.0327</th>
<th>71.0406</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_c$</td>
<td>0.5520</td>
<td>0.0583</td>
<td>0.0738</td>
<td>0.2915</td>
<td>0.0213</td>
<td>0.0030</td>
</tr>
<tr>
<td>$c$</td>
<td>0.0000</td>
<td>0.5929</td>
<td>0.3820</td>
<td>0.0098</td>
<td>0.0008</td>
<td>0.0145</td>
</tr>
<tr>
<td>$K_h$</td>
<td>0.0002</td>
<td>0.1064</td>
<td>0.4818</td>
<td>0.1752</td>
<td>0.1165</td>
<td>0.1199</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>0.0000</td>
<td>0.0004</td>
<td>0.0040</td>
<td>0.7829</td>
<td>0.1827</td>
<td>0.0300</td>
</tr>
<tr>
<td>$\alpha_T$</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0002</td>
<td>0.0031</td>
<td>0.5709</td>
<td>0.4258</td>
</tr>
<tr>
<td>$S_s$</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0001</td>
<td>0.613</td>
<td>0.9387</td>
</tr>
</tbody>
</table>

5.2.8 General discussion and conclusions on the Houtave test site

The forced gradient tracer test on the Houtave test site was used to demonstrate the benefits of the test and to provide real world data to test the newly developed software TRACER3D. It has been shown that with TRACER3D and HYPARIDEN, a forced gradient tracer test can be modelled successfully. With the sensitivity analyses, the benefits of the test have been shown. Both the hydraulic and the solute transport parameters can be derived and they are derived more accurately than is the case when one set of data (drawdown or concentration) is used. Layered heterogeneity is far more important than lateral heterogeneity here, and in this case, it was shown that pumping test data are in agreement with tracer test data.

A pumping and tracer test performed at the Houtave test site illustrates that proper analysis of both leads to coherent results. This is demonstrated by the successful prediction of the maximum breakthrough times in two observation points using hydraulic parameters derived from the pumping test. The important step herein is the careful interpretation of the pumping test in which the selection of the proper model is very important. The importance of this selection is illustrated by the interpretation of the pumping test with different models, on the one hand using the most frequently applied interpretation methods based on the models of Theis, Jacob, Jacob-Hantush and Boulton-Cooley and on the other hand using the program package HYPARIDEN (Lebbe, 1999a) which allows a flexible schematisation of the groundwater reservoir based on drilling descriptions and geophysical borehole logs. The results obtained with the HYPARIDEN program package are in good agreement with the tracer test using an acceptable value for the porosity. This is not the case with the results of the most frequently used interpretation methods which are derived from models in which the leakage from the adjacent semi-permeable layers is ignored or underestimated. Derived horizontal conductivities of the pumped layer are too large when the real leakage of the adjacent layers is underestimated in the models used during the interpretation.

The importance of the leakage in the Houtave test is shown in the sensitivities. During the interpretation of the drawdowns, hydraulic resistance from the pumping well is the second most sensitive parameter. The influence of leakage is further shown in figure 5.21. A cylinder is considered
centred around the pumping well with radius R. The relative discharge rate flowing through the upper and lower semi-permeable layer into the considered cylinder is calculated along with the discharge rate through the distal surface and the discharge originating from the storage decrease within the cylinder. All discharge rates are expressed in percentages of the total discharge rate. This was elaborated for a large number of coaxial cylinders with an increasing radius R or distance from the pumped well. The drawdowns calculated for the last time step, 24 hours after the start of the pumping test, are used. All water balances for these cylinders are considered in figure 5.21.

Close to the well, most water originates from horizontal flow in the pumped layer and the contribution of leakage is relatively small. This contribution becomes larger further from the pumping well. When considering a cylinder with radius of 42 m, the inflow by leakage from the lower semi-permeable layer equals the horizontal inflow. Due to the large hydraulic resistance of the peat layer, the contribution of leakage from this layer is relatively small. Water relieved from storage is limited due to the small value of the specific elastic storage and the relatively long time after the start of the pumping. Figure 5.21 shows that leakage in this case is very important and may not be neglected. This leakage will cause smaller drawdowns than in models without leakage or where the leakage is underestimated. Interpreting these smaller drawdowns with these models will result in horizontal conductivities for the pumped permeable layers that are too large. Figure 5.21 also shows that leakage becomes more and more important in function of distance from the pumping well. Using observation wells further from the pumping well will thus lead to larger errors when the leakage is neglected and consequently, the derived value for the horizontal hydraulic conductivity of the permeable layer will grow in function of distance. In case of a large leakage tracer breakthrough at a certain distance to the pumped well will be later than in the case of a small leakage. Coherent results of pumping and tracer test in dominantly layered heterogeneous media can only be obtained if the leakage is accurately evaluated in both models used for the interpretation of the tests. Large discrepancies are possible otherwise. One of these cases is illustrated by Niemann & Rovey (2000), who find that the horizontal conductivity derived with pumping test is 10 to 20 times larger than derived with tracer tests. These pumping tests were, however, interpreted with the Jacob semilog plot of time-drawdown data and with Theis type curve matching. Both interpretation methods are based on the Theis model where the leakage is completely ignored. Besides the influence of the heterogeneity, the major part of the discrepancy between the two tests will result from the ignorance of leakage.

![Figure 5.21](image)

**Figure 5.21** Relative discharge rate flowing through the upper, lower and distal surface of a cylinder, centred around the pumping well in the permeable layer and the relative amount of water originating from storage in the cylinder after 24 hours of pumping. The radius of the cylinder R varies from 0 to 350 m and the height equals the pumping well screen length.
Thorbjarnarson et al. (1998) derived with a pumping test an average horizontal conductivity for a layer 12.2 m in thickness. The groundwater reservoir was first studied with electrical conductivity logs of different wells and these results were incorporated into further analyses of pumping and tracer tests. With a tracer test, these authors are able to investigate layered heterogeneity within this layer and distinguish zones of 1 to 2 m in thickness for which hydraulic conductivity can be derived. They conclude that for the same time period, the highest permeability layer detected by the tracer test would predict six times larger solute movement than using an average conductivity. This illustrates our point of view that knowledge of layered heterogeneity is very important in both pumping test and tracer test analysis. This layered heterogeneity can be studied with drilling descriptions and geophysical borehole logs (for instance natural gamma log and electrical conductivity). The schematisation of the groundwater reservoir is made in function of the observed lithological variations. This layered heterogeneity can be inserted in HYPARIDEN resulting in a better modelling of the groundwater flow. With the inverse numerical model, hydraulic conductivity of individual layers can then be derived with a pumping test. Through careful planning of the observations to be made during the pumping test, variation of hydraulic conductivity can be distinguished in one layer, as illustrated here with the permeable layer for which hydraulic conductivity in the lower part is higher than in the upper part.

![Figure 5.22 Location of the Zevergem test site.](image)

5.3 Zevergem test site

5.3.1 Introduction

The Houtave test site proofed the concept of the forced gradient tracer test. Thereafter, a site with more heterogeneous sediments was sought. Therefore, a second test was performed in the quaternary Schelde deposits near the village of Zevergem (figure 5.22). A pumping test and a forced gradient tracer test were performed separately. The idea was to use two injection wells (IP1 and IP2), situated on both sides of a pumping well (PP) and observe the movement of the two tracer plumes towards the pumping well. This is referred to as a double forced gradient tracer test. Five observations wells were drilled (PB1 to PP5). It was planned to use a larger tracer plume as was the case at the Houtave test site. Due to this layout, a larger part of the aquifer was tested and it would be very interesting to see if...
both tracer plumes would behave in the same way. Hence, lateral heterogeneity and its influence on solute transport could be studied. A hydrogeological cross-section is shown in figure 5.23. Table 5.14 gives the lithological description based on rotary drillings. One pumping well and seven observation wells were drilled (table 5.15). In the boreholes, PVC tubes (inner diameter of 59 mm) with screen elements were installed. From bottom to top, the groundwater reservoir consists of an alternation of clay and silty sand (A), moderate to coarse sand (B), fine to moderate sand (C) and clay and sandy clay (D).

![Hydrogeological cross-section of the Zevergem test site. Numbering of layers as used in HYPARIDEN is shown at the right hand side. A: alternating clay and silty sand. B: moderate to coarse sand. C: fine to moderate sand. D: clay and sandy clay.]

**Figure 5.23** Hydrogeological cross section of the Zevergem test site. Numbering of layers as used in HYPARIDEN is shown at the right hand site. A: alternating clay and silty sand. B: moderate to coarse sand. C: fine to moderate sand. D: clay and sandy clay.

**Table 5.14** Lithological description of the Zevergem Test Site based on rotary drillings (De Bruyne, 2001).

<table>
<thead>
<tr>
<th>Depth (m)</th>
<th>Lithology</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0-0.4</td>
<td>Clay</td>
</tr>
<tr>
<td>0.4 – 1.3</td>
<td>Sandy clay</td>
</tr>
<tr>
<td>1.3 – 10.8</td>
<td>Fine to moderate sand with clay lenses</td>
</tr>
<tr>
<td>10.8 – 11.3</td>
<td>Moderate to coarse sand</td>
</tr>
<tr>
<td>11.3 – 12.3</td>
<td>Alternating clay and silty sand</td>
</tr>
<tr>
<td>12.3 – 12.4</td>
<td>Sand</td>
</tr>
<tr>
<td>12.4 – 13.3</td>
<td>Alternating clay and silty sand</td>
</tr>
<tr>
<td>13.3 – 13.4</td>
<td>Sand</td>
</tr>
<tr>
<td>13.4 – 14.7</td>
<td>Alternating clay and silty sand</td>
</tr>
</tbody>
</table>

**Table 5.15** Depth of screen interval (m) and distance (m) from pumping well PP for the different wells used for the pumping test.

<table>
<thead>
<tr>
<th>Well number</th>
<th>Screen interval (mTAW)</th>
<th>Distance to PP</th>
</tr>
</thead>
<tbody>
<tr>
<td>IP1</td>
<td>-1.35 – -3.35</td>
<td>7.5</td>
</tr>
<tr>
<td>PB1</td>
<td>-5.25 – -6.25</td>
<td>5.0</td>
</tr>
<tr>
<td>PB2</td>
<td>-5.05 – -6.05</td>
<td>2.5</td>
</tr>
<tr>
<td>PP</td>
<td>-1.65 – -5.65</td>
<td>/</td>
</tr>
<tr>
<td>PB3</td>
<td>-4.95 – -5.95</td>
<td>2.5</td>
</tr>
<tr>
<td>PB4</td>
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<td>5.0</td>
</tr>
<tr>
<td>IP2</td>
<td>-1.65 – -3.65</td>
<td>7.5</td>
</tr>
<tr>
<td>PP5</td>
<td>3.25 – 2.25</td>
<td>1.6</td>
</tr>
</tbody>
</table>
5.3.2 (Hydro)geological site characterisation

Natural gamma and EM39 logs are made. Natural gamma as logged in all wells is shown in figure 5.24. Top of the aquifer consists of a clay and sandy clay layer (layer D in fig. 5.23). This is a zone of high counts per second (cps) in the logs. The contact with the underlying fine to moderate sand (layer C) is undulating. This fine to moderate sand is present from 6.55 mTAW to –2.95 mTAW. Layered heterogeneity in layer C is present but not so obviously expressed. Lateral heterogeneity is more important. Zones of higher and lower clay content can be distinguished. Around 0 mTAW, a zone with a higher cps is seen. It is highly heterogeneous laterally. The part below 0 mTAW has a lower cps and shows also important lateral heterogeneity. Around –3 mTAW a zone, again highly heterogeneous laterally with a lower cps is seen. This is layer B. The contact with the underlying alteration of clay and silty sand is undulating. Although layered heterogeneity can be distinguished, lateral heterogeneity is more pronounced.

IP1 and IP2 are the injection wells used during the tracer test. The tracer will thus be injected in the base of layer C, layer B and the top of layer A. The middle of IP2’s screen is slightly less permeable then the upper and lower part. Towards PB3, clay content increases slightly, diminishing towards the pumping well. Clay content rises constantly towards the pumping well in layer C starting from IP2, so permeability will diminish towards the pumping well. In fact, this more sandy layer is far more clayey between IP2 and PP than between IP1 and PP. Between the latter, only from PB2 towards PP, layer C becomes slightly more clayey. The middle of the IP1 screen has a slightly higher clay content than the upper and lower part. Only between IP1 and PB1, small lateral heterogeneities can be seen. In layer A, a zone of higher cps is observed between PB3 and PB2. The sediments through which the tracer plume injected in IP2 will travel, is generally more heterogeneous than the sediments through which the tracer plume injected in IP1 will travel. Additionally of importance is a continuous sandy layer which is present between IP1 and PP and not between IP2 and PP.

Figure 5.24 Cross-section through the Zevergem Test Site based on the natural gamma logs (left) and EM39 (right). Vertical scale is the depth in mTAW.

Figure 5.24 shows also the EM39 logs in all wells. The groundwater reservoir is completely filled with water of the same quality. The pore water is a fresh F2 CaHCO$_3$+ water type (De Bruyne, 2001) following the classification of Stuyfzand (1986) with a total dissolved solid content (TDS) of 672 mg/L. This means that variations in measured electrical conductivity are due to lithological variations. A larger conductivity means a larger clay content and thus also a smaller hydraulic conductivity. The influence sphere of the EM39 measurement is larger than that of the natural gamma measurement. Heterogeneity can therefore not be studied in such a detail with the EM39. The relative response function of the EM39 makes the measurements far more sensitive for layered then for lateral heterogeneity if the conductivity contrast is small. Some general information which supplement the
natural gamma logs can be discerned. It can for instance be clearly seen that a less permeable layer is present around 0 mTAW.

5.3.3 Pumping test

Before the injection of the tracer, a pumping test was performed. During 43 hours, water was extracted from the pumping well PP with a discharge rate of 74.5 m³/d. Initially, all wells show the same potentiometric elevation coinciding with the water table. The water table is present 0.5 metre below surface level. No important natural horizontal and vertical gradients occur. Further, no recharge boundaries (lakes, streams, etc.) are present in the vicinity of the site. Drawdowns were measured with pressure probes in observation wells IP1, PB1, PB2, PB3, PP5 and IP2. The discretisation of the groundwater reservoir used in HYPARIDEN is shown in figure 5.23. Fourteen layers are considered. Layers 1 to 4 are the alternation of clay and silty sand (A). Layer 5 is the sand layer (B). Layers 6 to 13 are the fine to moderate sands (C) and layer 14 is the clay and sandy clay layer (D). Drawdowns measured in PB1, PB2 and PB3 are observations in layer 2, PB5 in layer 11 and IP1 and IP2 in layer 5. Pumping occurred in layers 3 to 7. The ratio of the discharge rate in each of these layers to the total discharge rate is set equal to the ratio of the transmissivity of each of these layers to the total transmissivity of layers 3 to 7.

Four different groups of parameters are deduced. The first group is the horizontal hydraulic conductivities of layers 1 to 14 (indicated further as $K_h(1-14)$). Horizontal conductivities of all fourteen layers are taken as one parameter group. Layered heterogeneity in these conductivities is included. This is done by the estimation of relative conductivities of the layers 1-4, layer 5, layer 6-13 and layer 14. The conductivity is 8.55 m/d for layers 1-4, 24.01 m/d for layer 5, 10.92 m/d for layers 6-13 and 0.30 m/d for layer 14. The second group is the specific elastic storages of layers 1 to 14 ($S_s(1-14)$). The specific elastic storage for layers 1-13 is $0.921 \times 10^{-4}$ m$^{-1}$ and $0.129 \times 10^{-3}$ m$^{-1}$ for layer 14. The third group is the hydraulic resistance of layers 1 to 14 excluding layer 9 ($c(1-13)$). The derived values result in an anisotropy or ratio of horizontal to vertical conductivity of 6.21. The hydraulic resistance of layer 9 ($c(9)$) is the fourth parameter. Its value is 7.14 d. The more clayey horizon that is present around 0 mTAW is modelled as a horizon with the hydraulic resistance $c(9)$. The storage coefficient near the water table is held at 0.04 during the interpretation. This parameter is not identifiable because the observations are insensitive for it. Table 5.16 shows the marginal and conditional standard deviation for the parameter groups. These parameter groups are arranged according to their sensitivity. The horizontal conductivities are the most sensitive parameters and are derived most reliably. Specific elastic storage is the second most sensitive parameter followed by the hydraulic resistances. Further, no large correlations between parameter groups are present (table 5.17). Condition indexes (table 5.18) are indicating only weak dependencies between parameters. Figure 5.25 shows the comparison between observed and calculated drawdowns.

### Table 5.16 Marginal $s_{m_j}$ and conditional $s_{c_j}$ standard deviation of the derived parameter groups during the pumping test analyses.

<table>
<thead>
<tr>
<th>Parameter Group</th>
<th>$s_{m_j}$</th>
<th>$s_{c_j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(1-14)$</td>
<td>0.0040</td>
<td>0.0027</td>
</tr>
<tr>
<td>$S_s(1-14)$</td>
<td>0.0222</td>
<td>0.0128</td>
</tr>
<tr>
<td>$c(9)$</td>
<td>0.0223</td>
<td>0.0038</td>
</tr>
<tr>
<td>$c(1-13)$</td>
<td>0.0391</td>
<td>0.0352</td>
</tr>
</tbody>
</table>

### Table 5.17 Partial correlation coefficients for the optimal parameter values.

<table>
<thead>
<tr>
<th>Parameter Group</th>
<th>$K_h(1-14)$</th>
<th>$S_s(1-14)$</th>
<th>$c(9)$</th>
<th>$c(1-13)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(1-14)$</td>
<td>1.0000</td>
<td>-0.8237</td>
<td>0.5259</td>
<td>-0.1211</td>
</tr>
<tr>
<td>$S_s(1-14)$</td>
<td>-0.8237</td>
<td>1.0000</td>
<td>-0.6807</td>
<td>0.1948</td>
</tr>
<tr>
<td>$c(9)$</td>
<td>0.5259</td>
<td>-0.6807</td>
<td>1.0000</td>
<td>-0.2784</td>
</tr>
<tr>
<td>$c(1-13)$</td>
<td>-0.1211</td>
<td>0.1948</td>
<td>-0.2784</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

83
Table 5.18 Condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportions due to the concentration observations.

<table>
<thead>
<tr>
<th></th>
<th>1.0</th>
<th>5.3</th>
<th>12.9</th>
<th>9.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(1-14)$</td>
<td>0.3024</td>
<td>0.1092</td>
<td>0.4834</td>
<td>0.1050</td>
</tr>
<tr>
<td>$S_z(1-14)$</td>
<td>0.0003</td>
<td>0.1156</td>
<td>0.7612</td>
<td>0.1229</td>
</tr>
<tr>
<td>$c(9)$</td>
<td>0.0000</td>
<td>0.1978</td>
<td>0.7616</td>
<td>0.0406</td>
</tr>
<tr>
<td>$c(1-13)$</td>
<td>0.0000</td>
<td>0.0028</td>
<td>0.2916</td>
<td>0.7056</td>
</tr>
</tbody>
</table>

Figure 5.25 Comparison between the observations (crosses) made during the pumping test and the calculations (full line) based on the derived optimal parameter values.
Although the horizontal conductivities are reliably derived, an estimation of their mutual ratios between $K_h(1-4)$, $K_h(5)$, $K_h(6-13)$ and $K_h(14)$ had to be made. Because the used observations are insensitive to $K_h(14)$, this parameter is not further considered in the discussion. The ratios $K_h(1-4)/K_h(5)$ and $K_h(1-4)/K_h(6-13)$ are respectively 1/2.81 and 1/1.28. Based on the natural gamma logs, layers 1 to 4 have the smallest conductivity and layer 5 the largest. The ratios of the conductivities are altered to see the effects on the optimal parameter values (table 5.19). In a last calculation, the conductivities of all layers are set equal. From table 5.19 it can be derived that the resulting conductivities of layers 1 to 4 and of layers 6 to 13 do not alter considerably. This is not the case for $K_h(5)$, the horizontal conductivity of a relatively thin part of the sequence. It can vary very much (from 10 to 24 m/d) without altering the optimal values of the conductivities of the other layers considerably.

### Table 5.19 Possible optimal values for $K_h(1-4)$, $K_h(5)$ and $K_h(6-13)$. The ratio $K_h(5)/K_h(1-4)$ and $K_h(6-13)/K_h(1-4)$ are indicated.

<table>
<thead>
<tr>
<th>$K_h(1-4)$</th>
<th>$K_h(5)$</th>
<th>$K_h(6-13)$</th>
<th>$K_h(5)/K_h(1-4)$</th>
<th>$K_h(6-13)/K_h(1-4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.55</td>
<td>24.01</td>
<td>10.92</td>
<td>1/2.81</td>
<td>1/1.28</td>
</tr>
<tr>
<td>8.89</td>
<td>17.80</td>
<td>11.37</td>
<td>1/2.00</td>
<td>1/1.28</td>
</tr>
<tr>
<td>9.10</td>
<td>13.64</td>
<td>11.62</td>
<td>1/1.50</td>
<td>1/1.28</td>
</tr>
<tr>
<td>7.94</td>
<td>22.46</td>
<td>11.91</td>
<td>1/2.81</td>
<td>1/1.50</td>
</tr>
<tr>
<td>10.57</td>
<td>10.57</td>
<td>10.57</td>
<td>1/1</td>
<td>1/1</td>
</tr>
</tbody>
</table>

To illustrate this point further, sensitivities are calculated as was done in section 5.2.6. Sensitivities were calculated for the position of observation wells PB2 (or PB3), PB1 (or PB4) and IP1 (or IP2) for the parameters $K_h(1-13)$, $K_h(1-4)$, $K_h(5)$ and $K_h(6-13)$ (figure 5.26). The sensitivity factor was $10^{0.1}$. The observations are very sensitive to $K_h(1-13)$, the conductivity of all layers (without layer 14) taken as one group. Although IP1 and IP2 are placed in layer 5, the observations are least sensitive for the conductivity of this layer resulting in small absolute values of sensitivity. This means that the conductivity can vary between large margins without considerable influence on other parameters during the parameter identification process. The observations are most sensitive to $K_h(1-4)$. Along with the insensitivity of $K_h(5)$, this means that the derived conductivity will not vary much by altering the mutual ratios. Sensitivities of all but the PB5 observations for $K_h(6-13)$ grow with time. The PB5 observations are very sensitive for the conductivities of layer 6-13.

![Figure 5.26 Sensitivity of observations made in PB1 (or PB4), PB2 (or PB3), PB5 and IP1 (or IP2) for the hydraulic conductivity of layers 1-13, layers 1-4, layer 5 and layers 6-13. Some examples of possible solutions these hydraulic conductivity are given below.](image-url)
If $K_h(1-4)$ and $K_h(6-13)$ are derived separately with HYPARIDEN, 9.22 m/d for the former and 10.39 m/d for the latter are found. These values depend, however, on the value for $K_h(5)$ which can alter them slightly. Due to these sensitivities, the best solution obtained during the interpretation of the pumping test is to estimate their ratios as was done. Based on only drawdown measurements, this leaves large uncertainties for $K_h(5)$, the most conductive layer of the site and thus a preferential pathway for solute transport.

To conclude, notice on figure 5.25 that the drawdown observations made in IP1/IP2 and in PB2/PB3 are made in the same layer and at the same distance from the pumping well. Despite this, they differ considerably. The reason for this is lateral heterogeneity. Main aim of the double forced gradient tracer test is now to derive hydraulic conductivities more in detail and to study the (lateral) heterogeneity.

### 5.3.4 Double forced gradient tracer test

#### 5.3.4.1 Presentation of observations and qualitative analysis

A volume of 2 m$^2$ of water with a TDS of 21250 mg/l was injected in IP1 and IP2 each. After the injection, pumping on PP was started and continued for 5 days. During this period, the observation wells were logged twice a day with the EM39 probe. Unfortunately, tracer breakthrough was very slow in PB3 and only the beginning of tracer breakthrough was observed. Measurement on the level of maximum tracer breakthrough in PB1, PB2, PB3 en PB4 are shown in figure 5.27. PB1 and PB4 are placed on an equal distance of respectively IP1 and IP2. If the groundwater reservoir is homogeneous and no important natural gradients are present, breakthrough in PB1 and PB4 should more or less at the same time. This is, however, not the case. Tracer breakthrough occurs after 54 hours in PB1 and after 102 hours in PB4. The same can be concluded from PB2 and PB3. So, the tracer injected in IP1 moves considerably faster than the tracer injected in IP2. No important natural gradients occur on the site, thus this must be due to aquifer heterogeneity. On the natural gamma log, it could be seen that the horizon in which the tracer plumes were injected was very heterogeneous. The zone between the pumping well and IP2 was thereby more clayey and sand layer was present between the pumping well and IP1. The result of this heterogeneity can also be seen in the tracer tests data.

![Figure 5.27 EM39 measurements on the level of maximum tracer breakthrough in PB1, PB2, PB3 en PB4.](image)
Figure 5.28 EM39-observations in PB1, PB2, PB3 and PB4 during the tracer test on different times after the start of the test (indicated in hours).

All observations are shown in figure 5.28. In PB1 and PB2, tracer breakthrough mainly occurs around –4 mTAW. A second horizon of tracer breakthrough can be seen in PB1 around –2.5 mTAW. Conductivity of the latter is much smaller and is retarded. In PB4 and PB3, tracer breakthrough occurs also mainly on –4 mTAW. In PB4 an important second breakthrough horizon can be seen on –2 mTAW.

Tracer breakthrough curves can be studied on different levels in the observation wells. This is presented here by the relative times of maximum breakthrough. For every level in which the tracer moves, the time of maximum concentration $T_i$ is determined and the mean time $T$ is calculated. Figure 5.29 shows the ratio $T/T_i$ for the different levels in PB4 and PB3. If $T/T_i$ is larger than 1, the time of tracer breakthrough is less than average and the horizontal conductivity is larger than average. If $T/T_i$ is less than 1, the time of tracer breakthrough is larger than average and the horizontal conductivity is less than average. Therefore, with such profiles vertical heterogeneity can be studied and individual layers can be identified within an apparent homogeneous unit. Only data from PB1 and PB2 can be used here. Not all individual breakthrough curves from PB4 and from PB3 show the time of maximum tracer breakthrough. If layers are lateral homogeneous, then the same profiles should be derived in different observation wells. This is, however, not the case, which confirms that the layer in which the
tracer is injected, is quite heterogeneous. In PB1 between –3 and –4.5 m TAW, a zone of larger hydraulic conductivity can be seen. This is however not the case in PB2. In PB2 an upper part with a somewhat smaller hydraulic conductivity and the lower part, with a somewhat larger hydraulic conductivity is found. The range of $T/T_i$ is larger than found on the Houtave Test Site (0.95-1.1). This demonstrates again the heterogeneous character of the deposits.

![Figure 5.29](image)

**Figure 5.29** Relative time of maximum tracer breakthrough in function of depth for PB4 and PB3.

### 5.3.4.2 Interpretation with TRACER3D

With the program package TRACER3D, the double forced gradient test was simulated. To link observed electrical conductivities to TDS, the formation factor must be known. The bulk conductivity of the sediments is 15.2 mS/m and the conductivity of the pore water is 58.5 mS/m. Hence, the formation factor is 3.85.

The discretisation of the groundwater reservoir used for interpretation of the pumping tests is the basis for the discretisation of the groundwater reservoir in TRACER3D. Layers 2 to 8 are further subdivided to simulate solute transport more accurately. This subdivision is given in table 5.20. In total, 28 layers are considered. As a starting point, the hydraulic parameters derived with the pumping tests are used after recalculation of the hydraulic resistance to the new layer thickness. As tracer movement between IP1 and PP and IP2 and PP is different, these parameters will be altered during the calibration of the model for either situation. The movement of each tracer plume is thus simulated separately.

Injection of the tracer is modelled two-dimensionally. The cross-section is 6.5 m high and has a width of 4 m. The injection well is placed centrally. Particle in-between distance of 5 cm is used. In this way, the model starts with 9469 particles and 28872 particles are generated throughout the calculations. During 3.0 h, the tracer is injected with a rate of 14.88 m³/d, or 1.9 m³ of tracer is injected. This period was divided in 73 timesteps. This relatively large amount of steps was needed to fulfil the stability criteria which are built into the model. During the short time span of injection, groundwater velocities change rapidly. The velocities must also be calculated very accurately very close to the axis of the pumping well. Initial radius is therefore 0.001 metre and the initial time is 0.1 minute. The distribution of the tracer around the injection well is thereafter used as starting point for the simulation of the tracer test. Background concentration is 672 mg/l, TDS of the tracer is 21250 mg/l.
First the movement of tracer plume injected in IP1 is modelled. A box with a surface of 11 x 3.0 m² and a depth of 5 m is placed around the pumping, injection and observation wells. Therein, particles are placed with an in-between distance of 10 cm. Around the injection well a second box of 3 x 3 x 5 m³ is considered wherein particles are spaced with an in-between distance of 5 cm. The model is run over 167 hours in 40 time steps. 231073 particles are used in the model. EM39 observations are calculated on the position of observation wells PB1 and PB2. First, the model was calibrated for the hydraulic conductivity and the porosity. The hydraulic conductivity of the pervious layer in which the tracer was injected, could not be uniquely determined from the drawdown observations only. Conductivity and porosity both determine the time of maximum tracer breakthrough concentration. Therefore, pumping and tracer test had to be interpreted iteratively. If the tracer test could be modelled with one value for the porosity and a certain variation in the conductivities, these must also reproduce the drawdown observations and vice versa. The optimal values derived with the pumping test given in section 5.3.3 are the final solution fitting both drawdown and concentration observations. From the modelling of the IP1 tracer plume, the optimal value for the porosity is 0.38 and the optimal value for horizontal conductivity of the permeable sand layer is 23 m/d. The longitudinal dispersivity is 0.08 m and the lateral dispersivity is 0.008 m. The ratio of longitudinal to transverse dispersivity is fixed at 10 for all the calculations because the observations are insensitive to this ratio. The calibration for PB1 is shown in figure 5.30. With these dispersivity values, however, the calculated concentrations for PB2 are larger than observed. To match the observations of PB2, longitudinal dispersivity of 0.17 m and lateral dispersivity is 0.017 m are needed. These are the only parameter values which must be changed. Figure 5.31 shows thus the comparison between observations and calculations in PB2.

### Table 5.20 Discretisation of the groundwater reservoir for TRACER3D

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness in HYPARIDEN (m)</th>
<th>Thickness in TRACER3D (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.9</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.3</td>
</tr>
<tr>
<td>7</td>
<td>0.7</td>
<td>0.25</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.25</td>
</tr>
<tr>
<td>6</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.2</td>
</tr>
<tr>
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<td>0.5</td>
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</tr>
<tr>
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<tr>
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</tr>
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<td></td>
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<td>0.2</td>
</tr>
<tr>
<td>3</td>
<td>0.9</td>
<td>0.9</td>
</tr>
<tr>
<td>2</td>
<td>1.1</td>
<td>0.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.7</td>
</tr>
</tbody>
</table>
Figure 5.30 Comparison of the concentration observations (dots) made PB1 during the double forced gradient tracer test and the calculations with TRACER3D. Horizontal axis is the concentration (mg/l), the vertical axis is the depth (mTAW).
Figure 5.31 Comparison of the concentration observations (dots) made in PB2 during the double forced gradient tracer test and the calculations with TRACER3D. Horizontal axis is the concentration (mg/l), the vertical axis is the depth (mTAW).

For the simulation of tracer movement from IP2 towards the pumping well, the same schematisation is used as for IP1. First, tracer breakthrough around –4 mTAW was modelled with a longitudinal dispersivity of 0.28 m and a lateral dispersivity of 0.028 m. The hydraulic conductivity for layers A and B is 9 m/d and is 10 m/d for layer C. Around –2 mTAW, a horizon with a conductivity of 6 m/d is needed to model the breakthrough on this level. With a longitudinal dispersivity of 0.28 m, it was impossible to simulate breakthrough around level –2 mTAW. The observed concentrations were too high. Therefore, different simulations were run with other dispersivity values. Tracer breakthrough could only be simulated when only advective transport is considered around the level –2 mTAW and both advective and dispersive transport with longitudinal dispersivity of 0.28 m and lateral dispersivity of 0.028 m for the rest of the tracer plume. Figure 5.32 shows the comparison between observations and calculations in PB4. Observations made in PB3 are not used in the calibration because maximum tracer breakthrough was not observed.
Hydraulic conductivity of the layers was also altered in comparison with the IP1 situation. In the latter a high conductivity zone of 24 m/d is found in which most of the tracer moves. This zone is not found with the second tracer plume. Hydraulic conductivity is the same for most of the groundwater reservoir (about 9 m/d) except a layer of lower conductivity around –2 mTAW (about 6 m/d). Around IP2 on this level, however, no zone of smaller hydraulic conductivity was found with the natural gamma logs. Between PB3 and the pumping well, such zone is present. This lateral heterogeneity can not be included in the model, hence a layer of lower conductivity is found. A résumé and comparison of the conductivity values found with the pumping test and the double forced gradient tracer test are given in figure 5.33.

5.3.5 Discussion and conclusion

The main advantage of a forced gradient tracer test is that both drawdown and concentration observations can be used to calibrate a model. One data set provides additive information for the other. The net result is that more parameters can be derived and also more accurately. This is clearly demonstrated on the Zevegem test site. The sandy deposits are characterised by a medium to high level of heterogeneity. Using only drawdown measurements, the conductivity of the most permeable layer on the site could not be derived. Generally, these horizons are the most important ones concerning solute transport. In the context of solute transport, contaminant or remediation studies, the
knowledge of its conductivity is therefore crucial. A tracer was injected in this layer. Adding concentration observations to the drawdown observations, the variation of conductivity in layer B could be studied and parameter values were derived.

![Figure 5.33](image)

**Figure 5.33** Comparison of the hydraulic conductivity profile derived with the pumping test using all wells and tracer test using wells PB1 and PB2 and well PB4.

Natural gamma logs in the wells showed that the groundwater reservoir in general and layer B in particular is moderately to strongly heterogeneous, both layered and lateral heterogeneity occurs. Therefore, two injection wells on either side of the pumping well were used to investigate if differences in tracer movement would occur and if these differences could be brought in relation to aquifer heterogeneity. The tracer injected in IP1 was advancing faster to the pumping well. Modelling with TRACER3D showed that the plume was moving in a layer with a hydraulic conductivity of 24 m/d. The tracer injected in IP2 was moving slower. The hydraulic conductivity of layer B is in this case 9 m/d. Additionally, there is a zone around –2 mTAW with a conductivity of 6 m/d wherein the tracer moves slower. These differences were observed on a cross section made with natural gamma logs in all wells.

No single value for the dispersivity is derived. Only longitudinal dispersivity could be studied because the observations were insensitive to transverse dispersivity. The ratio of longitudinal to transverse dispersivity is therefore fixed at 10. Longitudinal dispersivity for PB1 and PB2 are respectively 0.08 and 0.17 m. In observation well PB4 longitudinal dispersivity of the bulk of the tracer plume is 0.28 m. The upper part of the tracer moved in a less conductive horizon for which no dispersivity was needed to model the observations. Reason for this different behaviour is aquifer heterogeneity, however, reasons for this particular case can not be readily found in drilling description or borehole measurements. Figure 5.34 shows a sediment description in a nearby quarry (Heyse, 1979). L2 to L5 are the same sediments which are found at the Zevergem test site (Heyse, pers. com.). L2 to L4 consists of gullies cut by the quarry face at different angles. Individual gullies are 3 to 20 m in cross-section. Sedimentation in these gullies is not uniform. These layers poses thus an important layered as well as lateral heterogeneity resulting in the dispersivity values found with the tracer test. It can also explain the different behaviour of the two tracer plumes. In L5, layered heterogeneity is by far more important than lateral heterogeneity. Dispersivity along these layers will be small. It could be possible that this is a similar type of horizon which is observed with the upper part of the IP2 plume. Indeed, only advective transport was used to model this part of the tracer plume.
5.4 Tessenderlo test site: towards an application

5.4.1 Introduction

At a field site in Tessenderlo, a pumping test and a forced gradient tracer test were performed. Instead of pure scientific and experimental motives, the tests done on the Tessenderlo test site had a practical purpose. The site is contaminated by 1,2-dichloroethane (1,2-DCA) and a remediation scheme had to be developed. A bacteria, Desulfitobacterium dichloroeliminans strain DCA1, was identified at the Laboratory for Microbial Ecology and Technology (LabMET) of Ghent University. Strain DCA1 can detoxify 1,2-DCA quickly in anaerobic circumstances without producing other hazardous products (De Wilde man, 2002). With the pumping and tracer test solute transport and hydraulic parameters were derived to characterise the test site, plan further in situ tests and ultimately to develop a remediation scheme. This context will be discussed further in chapter 7. Here, the interpretations of the pumping and tracer test are discussed.

The site is situated on figure 5.35. Figure 5.36 gives a cross-section through the site. The first 1.5 m consists of sandy clay. Below it, moderate fine to clayey glauconite sand and clayey moderate fine glauconite sand with sandstone fragments is found. Three observations wells were drilled, LV22A,
LV22B and LV51 (outer diameter of casing is 63 mm). LV22A and LV22B are two separate observation wells placed next to each other. Two injection/pumping wells were drilled, LV50 and LV52 (outer diameter of casing is 125 mm). The sediments are of tertiary age and the site is situated at the southern edge of the North Sea Basin, a complex of NNE dipping subhorizontal sand, clay and chalk layers. The glauconite sands of the Tessenderlo test site are the top layers of the Diest Formation. These deposits are of Miocene age. The deposits have a thickness of about 110 m at Tessenderlo and are part of an important erosive gully in the underlying clay of the Boom Formation. This severe erosion was the result of a lowering of the sea level and an uplift of the Brabant Massif. Deposits of the Diest Formation consist of migrating sandbanks.

![Location of the Tessenderlo test site.](image)

**Figure 5.35** Location of the Tessenderlo test site.

![Schematical cross-section of the Tessenderlo test site. Graph at the left hand site is the EM39 conductivity (mS/m) measured in LV51. Sediment descriptions are from the drilling firm.](image)

**Figure 5.36** Schematical cross-section of the Tessenderlo test site. Graph at the left hand site is the EM39 conductivity (mS/m) measured in LV51. Sediment descriptions are from the drilling firm.
Figure 5.36 shows also an EM39 measurement made in observation well LV51. Only minor variations of the electrical conductivity can be seen below the water table. A clear division at a depth of 12 m can be seen dividing a zone of smaller conductivity below it from a zone with gradually increasing conductivity with depth above it. Just below the water table, the conductivity is also smaller.

5.4.2 Step drawdown test

A step drawdown test is a pumping test whereby the discharge rate is altered during the course of the test. Typically, four steps are used. Discharge rate is small during the first step and is increased in the following three steps. A step drawdown test has the advantage over an ordinary pumping test that well characteristics of the pumping well can be studied, if drawdowns are also measured in it. Drawdowns in a pumping well are due to aquifer loss and well loss. Aquifer loss is the drawdown that would occur at the borehole wall situated at the same depth interval of the well screen if the pervious layer just outside the borehole wall is unaltered and has the same hydraulic parameters as the rest of the aquifer. The well loss is here defined as the difference between the drawdown in the pumping well and the aquifer loss. It is the result of different flow phenomena that occur in the vicinity and inside the pumped well: for instance the flow inside the pumping well towards the pump intake, the flow through the well screen and filter pack and the flow through the borehole wall and immediate surroundings. The well efficiency is the ratio of the aquifer loss to the drawdown in the pumped well expressed as a percentage. This well efficiency can alter in time, for instance by clocking of the well screen. Before the performance of the pumping and tracer test, it was known that water with bacteria, a carbon source and perhaps other chemicals would be injected in the pumping well LV50 in the future. It was therefore interesting to see if these injections have any influence on well efficiency (for instance clocking of the well screen) thinking on the design of a workable remediation set up. To keep this possibility, it was decided to perform a step drawdown test instead of a normal pumping test.

The aquifer loss is calculated directly by the numerical model. This must be increased with the well loss to obtain the drawdown in the pumping well. The well loss is assumed to be proportional to the power \( N \) of the discharge rate or equal to \( CQ^N \) (Todd, 1980). The \( C \) value is the well loss function constant. \( N \) is a constant greater than one and Jacob (1947) suggested that \( N=2 \) might be reasonably assumed. Rorabaugh (1953) pointed out that the power \( N \) can deviate significantly from 2. An exact value for \( N \) cannot be stated because of differences of individual wells. \( C \) and \( N \) are values that can be included in HYPARIDEN.

Figure 5.36 shows the layers used in the numerical model. The groundwater reservoir is subdivided in 17 layers. Bottom of the ground water reservoir is the clay of the Boom Formation which is considered as impervious in this study. It is found approximately 107.5 metres below surface level. Hydrogeological information on the sediments from the Diest Formation is taken from a study on these sediments at Beerse, Rijkevorsel and Merksplas (Lebbe & De Breuck, 1979). The upper part of the Diest Formation is heterogeneous. It is an alternation of fine to moderate fine sands with varying silt content. Below it, well sorted moderate fine sands are found. The bottom of the Diest Formation consists of fine sands. There is thus a gradual coarsening upwards. Layers 1 to 5 are part of the Diest Formation, having gradually smaller conductivities deeper in the groundwater reservoir. Layers 7 to 16 are the upper heterogeneous part of the Diest Formation. Thickness of all layers is found in table 5.21. The water table is situated approximately 6.5 metre below land surface. Initially, all wells show the same potentiometric elevation coinciding with the water table. No important natural horizontal and vertical gradients occur. Further, no recharge boundaries (lakes, streams, etc.) are present in the vicinity of the site. LV50 is the pumping well and is situated in layers 9 and 10. The step drawdown test consisted of four steps, each lasting 1.5 hour respectively with discharge rates of 46.8 m³/d, 96.0 m³/d, 144.0 m³/d and 198.0 m³/d. LV22B, LV51 and LV52 are situated in layer 10 and LV22A in 15. Two additional wells located in layer 10 at a distance of 44.2 and 52.8 m from the pumping well were used as observation wells. Drawdowns were measured in all wells, including the pumping well. Due to practical problems, only one measurement in LV22A was usable.
Table 5.21 Thickness of layers and optimal parameter values.

<table>
<thead>
<tr>
<th>layer</th>
<th>Thickness (m)</th>
<th>$K_h$ (m/d)</th>
<th>c (d)</th>
<th>$S_S$ (m$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32.0</td>
<td>0.50</td>
<td>88.26</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>2</td>
<td>24.0</td>
<td>1.00</td>
<td>31.87</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>3</td>
<td>16.0</td>
<td>2.00</td>
<td>9.95</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>8.0</td>
<td>4.00</td>
<td>2.49</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>4.0</td>
<td>8.00</td>
<td>1.50</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>6</td>
<td>2.0</td>
<td>2.00</td>
<td>1.50</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>7</td>
<td>1.0</td>
<td>2.00</td>
<td>0.74</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>8</td>
<td>0.5</td>
<td>2.00</td>
<td>0.74</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>9</td>
<td>3.5</td>
<td>7.06</td>
<td>0.77</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>10</td>
<td>3.5</td>
<td>12.8</td>
<td>0.31</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>11</td>
<td>0.5</td>
<td>12.8</td>
<td>0.12</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>12</td>
<td>1.0</td>
<td>12.8</td>
<td>0.16</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>13</td>
<td>1.0</td>
<td>12.8</td>
<td>0.16</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>14</td>
<td>1.0</td>
<td>12.8</td>
<td>0.16</td>
<td>0.100 10$^{-3}$</td>
</tr>
<tr>
<td>15</td>
<td>1.0</td>
<td>0.60</td>
<td>8.25</td>
<td>0.54 10$^{-4}$</td>
</tr>
<tr>
<td>16</td>
<td>1.0</td>
<td>0.60</td>
<td>24.76</td>
<td>0.54 10$^{-4}$</td>
</tr>
</tbody>
</table>

$S_0 = 0.16$  $C = 9.402 	imes 10^{-6}$  $N = 2.0$

Some remarks must be made with regard to the location of the wells. The observation wells have long screens. These are also situated in different layers. Additionally, no drawdowns were measured above (only one observation) or below the level of the pumping well. This is not ideal for a step drawdown test. Well emplacement was the result of available resources and the highest common factor of desiderata from the site owners, LabMET and the hydrogeologists. Result is that the site is optimised for the planned tracer test but not ideally suited for a pumping test. This is reflected in the parameters that could be optimised. Results of the tracer test had to be maximally incorporated in the interpretation of the drawdowns. Here, more than on the other two field site the interpretation of the drawdowns and concentrations was an iterative exercise. The optimal parameters given in table 5.21 are thus the end result of the combined interpretation. Three parameter groups are considered during the interpretation of the step drawdown test. The first group is the horizontal hydraulic conductivities of layers 1 to 17 along with their hydraulic resistances (further indicated as $K_h(1-17)$). Anisotropy or the ratio of horizontal to vertical conductivity is set at 2. Conductivity ratios between different layers had to be estimated since no further detailed information on them can be obtained from the observations. The second group is the specific elastic storage of layers 1 to 17 ($S_S(1-17)$). C-value ($C$) of the well loss is the third parameter. Other parameters, for instance the N-factor of well loss and the storage coefficient near the water table, are insensitive to the observations and are thus unidentifiable. Well efficiency is for the four steps respectively 98%, 94%, 91% and 87%. Tables 5.22 and 5.23 give the marginal and conditional standard deviation of the parameter groups, partial correlation coefficients for the optimal parameter values and the condition indexes and $\pi$ matrix of marginal variance-decomposition proportions. Hydraulic conductivity of the sediments is the most sensitive parameter. No important correlations between the identified parameters exist. The largest condition index is 26.9, indicating moderate dependencies between parameters (Belsley, 1990). Figure 5.37 shows the comparison between observed and calculated drawdowns.

Table 5.22 Marginal $s_m$ and conditional $s_c$ standard deviation of the parameter groups and partial correlation coefficients for the optimal parameter values. Parameters are arranged according to sensitivity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$s_m$</th>
<th>$s_c$</th>
<th>$K_h(1-17)$</th>
<th>$S_S(1-17)$</th>
<th>$C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(1-17)$</td>
<td>0.0050</td>
<td>0.0032</td>
<td>1.0000</td>
<td>-0.7258</td>
<td>0.5776</td>
</tr>
<tr>
<td>$S_S(1-17)$</td>
<td>0.0522</td>
<td>0.0079</td>
<td>-0.7258</td>
<td>1.0000</td>
<td>-0.3741</td>
</tr>
<tr>
<td>$C$</td>
<td>0.0763</td>
<td>0.0681</td>
<td>0.5776</td>
<td>-0.3741</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
Table 5.23 Condition indexes $\mu$ and $\pi$ matrix of marginal variance-decomposition proportion.

<table>
<thead>
<tr>
<th></th>
<th>1.0</th>
<th>15.5</th>
<th>26.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_h(1-17)$</td>
<td>0.3616</td>
<td>0.1650</td>
<td>0.4734</td>
</tr>
<tr>
<td>$S_h(1-17)$</td>
<td>0.0000</td>
<td>0.6700</td>
<td>0.3300</td>
</tr>
<tr>
<td>$C$</td>
<td>0.0000</td>
<td>0.0513</td>
<td>0.9487</td>
</tr>
</tbody>
</table>

Figure 5.37 Comparison between observed (crosses) and calculated (full line) drawdowns.

Figure 5.38 shows the sensitivity of the observations made in LV22A, LV22B, LV51 and LV52 for the horizontal hydraulic conductivity of layers 6-8, layer 9 and layers 9-15 and the hydraulic leakage of layers 6-8 and layers 9-15. It shows that the observations are sensitive to all these parameters. They are least sensitive to the conductivity and the leakage of layers 6-8. This is due to the fact that the observations wells are placed in the model layer 10. Actually, they are placed in layers 9 and 10 but this can not be modelled. Placing the observation wells in layer 9 does not alter the conclusion made here. Sensitivity analyses learn that the drawdown observations are sensitive to conductivities and hydraulic resistances of individual layers. They can, however, not be determined due to the long screens and their emplacement. Further information must come from concentration observations made during the tracer test.
5.4.3 Forced gradient tracer test

About 2.1 m³ water marked with NaCl was injected in LV50. TDS of the injection water was 10.8 g/l. After the injection, water abstraction from LV52 started. Discharge rate of 2.0 m³/d was constant during the test. Movement of the tracer was followed in two observation wells (LV22B en LV51). EM39 measurements were performed twice a day during a period of 12 days. Figures 5.39 and 5.40 show the observations in both observation wells. The largest conductivities are found in the lower part of the tracer plume in both observation wells.
Figure 5.39 EM39 observations in LV22B. Times are in hours after the start of the pumping in LV52.

Figure 5.40 EM39 observations in LV51. Times are in hours after the start of the pumping in LV52.

Tracer breakthrough curves can be studied on different levels in the observation wells. This is presented here by the relative times of maximum breakthrough. For every level in which the tracer moves, the time of maximum concentration $T_i$ is determined and the mean time $T$ is calculated. Figure 5.41 shows the ratio $T/T_i$ for the different levels in LV22B and LV51. When $T/T_i$ is larger than 1, the time of tracer breakthrough is less than average and the horizontal conductivity is larger than average. If $T/T_i$ is less than 1, the time of tracer breakthrough is larger than average and the horizontal conductivity is less than average. In both observation wells, hydraulic conductivity becomes smaller.
deeper in the ground water reservoir. Between 12 and 13 metre deep in LV22B, there is a zone where the hydraulic conductivity is also smaller. A similar zone is found somewhat deeper in LV51.

![Figure 5.41](image)

*Figure 5.41 Relative time of maximum tracer breakthrough in function of depth for PB4 and PB3.*

The forced gradient test was simulated with the program package TRACER3D. To link observed electrical conductivities to TDS, the formation factor must be known. This is not as straightforward here as it was on the other two field site. The deposits are glauconite and generally clay bearing. This means that the matrix resistivity cannot be ignored in equation 4.1. To recalculate bulk sediment conductivities to TDS values, the combination of formation factor and the matrix conductivity must be known (see section 4.1.4) here. This is, however, not the case. Formation factor cannot be derived from bulk sediment conductivity and pore water conductivity only because matrix conductivity cannot be ignored. An additional complication is the fact that matrix conductivity and formation factor will alter in function of clay content. To calculate TDS-values from the EM-39 measurements, it is assumed that pore water conductivity before the injection of the tracer is constant in the groundwater reservoir. This conductivity is 86 mS/m, corresponding with a TDS of 860 mg/l, a mean TDS of water samples extracted on the field site. Studies in the western part of the Belgian coastal plain have shown that the formation factor ranges between 2.7 and 5, most likely between 3.4 and 4.5 (Lebbe, 1978; Lebbe & De Breuck, 1994). Therefore, a constant formation factor of 4 is supposed. EM39 logs were made in the observation wells before the start of the tracer test. With this natural background conductivity (this is the bulk sediment conductivity), pore water conductivity of 86 mS/m and a formation factor of 4, the resulting matrix conductivity for every observation point is calculated. The EM39 logs made during the tracer tests are now recalculated with a formation factor of 4 and corresponding matrix conductivity. TDS in zones where the tracer is not (yet) present is thus 860 mg/l. Where the tracer is present, a TDS value for it is calculated. The background conductivity (see figures 5.39 and 5.40) increases in function of depth. The general trend in matrix conductivity is thus the same. Mean matrix conductivity in LV22B and LV51 are respectively 12.29 mS/m and 10.7 mS/m. These values are in the same order as results on fine grained sediments from the western part of the Belgian coastal plain (Lebbe & De Breuck, 1994) and the Gorleben site (Repsold, 1989).

The schematisation used in TRACER3D is based on the one used in HYPARIDEN albeit refined. The first three layers are combined in one layer of 72 m thickness. Starting from layer 9, the grid is refined. Successively from bottom to top, 2 layers of 0.5 m, 1 layer of 0.4 m, 19 layers of 0.3 m, 3 layers of 0.4, 3 layers of 1.0 m and 1 layer of 2.0 m thickness are used. A total of 35 layers is used. Hydraulic parameters derived from the pumping test were used as initial values. They are altered as the drawdown and concentration data are interpreted iteratively. Injection is modelled two-dimensionally. The cross-section is 7 m high and has a width of 4 m. The injection well is placed centrally. Particle in-between distance of 5 cm is used. In this way, the model starts with 13349 particles and 60060
particles are generated throughout the calculations. Water is injected with a rate of 48 m$^3$/d during 63 minutes, resulting in an injection volume of 2.1 m$^3$. The distribution of the tracer around the injection well is thereafter used as starting point for the simulation of the tracer test. Background concentration is 860 mg/l, TDS of the tracer is 10.8 g/l.

Next step is the simulation of the tracer movement. A box of 7.7 x 4.0 m$^2$ and a depth of 11 m is placed around the pumping, injection and observation wells. In this box particles are placed with an in-between distance of 5 cm. The model is run over 320 hours divided in 40 time steps. 631801 particles are used in the model. EM39 observations are calculated on the position of observation wells LV22B and LV51. Figures 5.42 and 5.43 give the comparison between observations and calculations in the observation wells. Figure 5.44 gives the horizontal conductivity in function of depth derived from the drawdown and concentration data. First, the conductivities derived from both data sets are in very

Figure 5.42 Comparison between observations (points) and calculations (full line) in LV22B. Times are in hours after the start of the pumping.
good agreement. It was found that the tracer plume moved in two layers with different conductivity. The upper layer (± layer 10 on figure 5.36) has a conductivity of 13.4 m/d. The lower layer (± layer 9 on figure 5.36) has a conductivity of 7.4 m/d. Further, the effective porosity is 0.37. To calibrate the observations made in LV22B, only advective transport is considered. Dispersion is too small to be important. However, a longitudinal dispersivity of 0.08 m is needed to model the observations made in LV51. Transverse dispersivity is fixed at 10 times smaller. Dispersivity increases thus also on this field site in function of travel distance of the tracer plume.

Figure 5.43 Comparison between observations (points) and calculations (full line) in LV51. Times are in hours after the start of the pumping.
5.4.4 Modelling the injection phase and the solute balance

Although the fit between observations and calculations is good, an important problem arises when the solute budget is made. During the calibration process, the distribution of the tracer around the injection well calculated with the 2D model is adjusted. This was also the case on the two other test sites and its implications will be discussed in section 5.5. However, in these cases the total volume of injected tracer was not altered. When for instance 0.5 m³ of water was injected on the Houtave test site, this volume was needed to model the observations. This was strangely enough not the case on the Tessenderlo test site. Figure 5.45 shows the distribution of the tracer around the injection well as is expected based on the 2D modelling and as was used during the calibration of the tracer test. A volume of 2.1 m³ was injected. Only 0.93 m³ is used in the model meaning that 1.17 m³ or 55.7% of the injected water is missing. The largest differences seen in figure 5.45 are situated in the upper part of the tracer plume. Less volume is needed around the injection well in the upper part to model the observations. The upper part has, however, a larger conductivity which means that the injection water should invade this zone deeper.

Figure 5.45 Distribution of the tracer around the injection well as was used during the calibration of the tracer test (1) and was expected based on the 2D modelling (2).
A number of reasons for this discrepancy can be quoted. Firstly, all breakthrough curves on individual levels in the vertical profiles exhibit tailing. Figure 5.46A is an example of a breakthrough curve (BTC) made in LV22B, 16.3 metre below surface level. Two important observations can be made. The calculated TDS values decrease more rapidly after maximum breakthrough. Additionally, the observed TDS values have not yet returned to their background value at the end of the test. These are observation which, in different levels of importance, can be seen on all depths. An important amount of tracer is thus dragging behind in a tail. The coefficient of skewness of the breakthrough curves is calculated in LV22B and LV51 (figure 5.46B). A positive skewness means that the breakthrough curve is skewed to the right or that a tail is present. In LV22B BTCs are positively skewed below 11.7 m. A division is present around 14.3 m. Above it, skewness is larger. This division is approximately on the same level as the transition between layer 9 ($K_h = 7.4$ m/d) and layer 10 ($K_h = 13.4$ m/d) in the numerical model. This same division is seen in LV51. However, below it skewness is positive, above it skewness changes chaotically between positive and negative values. This same chaotic behaviour is observed in LV22B above a depth of 11.7 m. The deepest part of the tracer plumes shows also chaotic varying skewness.

Thus, an important volume of tracer is present in a tail and moves only very slowly towards the pumping well. Coefficients of skewness in LV22B and LV51 show a number of zones coinciding with zones of different hydraulic conductivity. Differences between LV22B and LV51, mainly above 14.3 m, are due to lateral heterogeneity. Largest differences on the curve of relative maximum tracer breakthrough (figure 5.41) are also found on these levels.

![Figure 5.46 A: breakthrough curve 16.3 m below surface in LV22B. B: skewness in LV22B and LV51 in function of depth.](image)

Why then does an important amount of tracer stays behind? It was not observed on the other two test sites. The characteristic that sets the Tessenderlo site apart is the large amount of glauconite and varying clay content of the sediment. Part of the tracer plume may get stocked in clay lenses, retarding the distal part of the tracer plume considerably. A related possibility is that the hydraulic conductivity changes due to the passage of the salt water. Equation 5.8 gives the relation between the formation factor $F$ of sediment filled with fresh water and with pore water resistivity $\rho_w$ and the formation factor of sediments filled with salt water $F_0$ and pore water resistivity $\rho_{w0}$ (Hill & Milburn, 1957):

$$F = F_0 \left( \frac{\rho_w}{\rho_{w0}} \right) \ln \left( \frac{\rho_w}{\rho_{w0}} \right) \left( 0.135Q + 0.0055 \right)$$  \hspace{1cm} 5.8

$Q$ is the cation exchange capacity (meq/cm²). If fresh water is flushed by salt water and the cation exchange capacity of the sediments is important, than the formation factor will become larger. Following Archie (1942), the porosity $n$ will diminish:
where \( a \) is a proportionality factor and the power \( m \) is known as the sedimentation factor. A smaller porosity means a smaller conductivity. If conductivity becomes smaller after passage of the salt waters proximal part, the distal part will be delayed.

Secondly, some important assumptions are made in recalculating the EM39 observations to TDS values. They may be an important simplification of the actual situation. The formation factor and/or the matrix conductivity can be fundamentally different in different parts through which the tracer plumes moved, altering the observed TDS values. Although the EM39 TDS values are calculated in a logical way, some uncertainty about them remains.

### 5.4.5 Discussion and conclusions

The behaviour of a relatively large tracer plume could be followed and studied, identifying preferential pathways of tracer migration. Coupled with that, hydraulic and solute transport parameters were derived. Other tests with for instance bacteria could be planned more accurately (see further in chapter 7). This was the main goal of this test.

Pumping and tracer test showed very clearly the benefits of a combined interpretation of the drawdown and concentration measurements. The test site was developed to suite different goals. It was not ideally designed for a pumping test and parameters were thus derived with relatively large uncertainties. Concentration observations provided additional information to overcome this. Conductivities of the most important layers, porosity, dispersivity and specific elastic storage could be derived.

Important tailing was observed, unbalancing the mass budget of the model. Different reasons can be quoted. Clay lenses can retard parts of the tracer plume or passage of the tracer plume can have an effect on the hydraulic conductivity. More research on these topics, influence of the passage of salt water through glauconite rich sediments and clay, its influence on hydraulic conductivity, influences on electrical conductivity, is needed. Additionally, the calculations of TDS values from EM39 conductivities is not as straightforward as on the other two sites due to the influence of matrix conductivity. Matrix conductivity and formation factor can vary in the sediments making these recalculations complicated. The most reasonable but perhaps a little to simplified calculation was performed here. It points definitely to the fact that more research on this topic must be done. Probably no single reason will be responsible for the mass balance deviation.

### 5.5 Injection of the tracer

Until now, simulation of the injection phase was only briefly touched. It is simulated with a two dimensional axial-symmetric model in the program package TRACER3D. Injection water forms a cylinder around the injection well. The radius \( r \) (m) of this cylinder is dependent of the effective porosity \( n_e \), the volume of water injected (m³) and height of the screen \( h \) (m):

\[
r = \sqrt{\frac{V}{\pi \times n_e \times h}}
\]
If hydraulic conductivity varies over the depth of the screen, this must be taken into account. The radius is proportional to the ratio of the transmissivity of an individual layer to the total transmissivity over the screen interval. If \( n \) layers with horizontal conductivity \( K_{h,i} \) (m/d) and thickness \( b_i \) (m) are present, transmissivity (m²/d) of each layer is \( K_{h,i} \times b_i \) and total transmissivity is \( \sum_n K_{h,i} \times b_i \). The radius \( r_i \) (m) for layer \( i \) with thickness \( b_i \) is then:

\[
r_i = \frac{V \times K_{h,i}}{\sqrt{\pi \times b_i \times n_e \times \sum_n K_{h,i} \times b_i}}
\]

5.11

![Figure 5.47](image)

**Figure 5.47** Comparison between the expected and modelled distribution of tracer around the injection wells at the Houtave, Zevergem and Tessenderlo test sites.

This is simulated with the 2D model. For all test sites, these distributions had to be adjusted. Figure 5.47 shows a comparison between the expected, based on the assumption explained above, and eventually modelled distribution of tracer around the injection wells at the Houtave, Zevergem and Tessenderlo test site. The difference between the expected distribution based on the transmissivities and the one used in the model is noteworthy. The volume of actually water injected and used in the model, however, is approximately the same on the Houtave and Zevergem site. This was not the case on the Tessenderlo test site, due to a number of reasons discussed above. Focus is here therefore on the two other sites. On the Houtave test site, tracer is found over a wider depth interval than expected. This is balanced by a smaller radius of the injection cylinder. Tracer is found somewhat deeper around IP2 of the Zevergem test site. The lower part of the plume invades also deeper in the groundwater reservoir than expected. Around IP2, the tracer is also found over a larger depth interval and is present in two different horizons. These distributions are thus not correlated with transmissivity as given in equation 5.11. This transmissivity in the immediate surrounding of the well is, however, severely influenced by the drilling process and the emplacement of the well itself. Calibrated sand is present around the well screen and the sediments around it are distorted. This can severely alter the flow close to the injection well. This flow is of importance during the injection phase. Typically, tracer is found
deeper than expected. Wells are drilled somewhat deeper than the bottom of the well because some parts of the borehole wall will collapse in the time between the end of the drilling and emplacement of the well screens. These collapsed sediments are in most cases more conductive than the surrounding sediments and this forms an easy pathway for tracer migration. The drilling activity must also account for the other discrepancies. In IP2 for instance, drilling was stopped temporarily due to technical purposes. The well was actually drilled in two steps, influencing the transmissivity around the well resulting in the observed tracer distribution.

5.6 Push-pull tests

5.6.1 Introduction

One push-pull test was performed on the Houtave test site. An oxygenated test solution of NaBr and KNO$_3$ was injected. The aim of the test was to have a first acquaintance with this sort of tests and to see what kind of reactions would happen. Specifically aerobic respiration and denitrification due to the presence of the peat layer and organic content of the sediments were of interest. Additionally, first-order reaction rate coefficients could be derived. It would also be very interesting to see if aerobic respiration and denitrification could be observed with one test. Otherwise, two test should be used each with a specific tracer. A second push-pull test was performed on the Tessenderlo test site in the framework of the design of a remediation scheme. This second test will be discussed in chapter 7.

5.6.2 Push-pull test on the Houtave test site

PP5 on the Houtave test site (see figure 5.2) was used for a push-pull test. This well is situated directly under a peat layer in fine sandy deposits of quaternary age. These deposits also contain organic material. The sediments are present always below the water table, thus in suboxic to anoxic circumstances.

First 500 l of water was pumped from PP5 and collected in a metal container. The analysis of this formation water is given in table 5.24. This container was open to the air so that the water is saturated with oxygen. Then 5 l of a solution containing a tracer was added. This tracer solution consisted of about 130 g NaBr and 180 g KNO3 dissolved in water. Finally 271 l of this 505 l water marked by the tracer solution was injected in well PP5. The injection water is thus marked by bromide which is a conservative tracer, oxygen and nitrate that will react in successive steps with organic matter and sodium and potassium that could perhaps react in the groundwater reservoir. Oxygen and nitrate must allow us to see aerobic respiration and perhaps the successive denitrification. The injection was very short, about 30 minutes. After every 30 minutes for a period of 8 hours, about 26 l of water was pumped from PP5. This took only some minute’s time. Field measurements were made and water samples were taken. These pumping cycles give a mean discharge rate of 1.248 m$^3$/d. Some field measurements were made. Dissolved oxygen content, pH, and Eh were measured with electrodes in a flow cell to prevent air admission. Additionally, electrical conductivity is measured. The CO$_3^{2-}$ and HCO$_3^-$ concentrations are determined by titration respectively as the fenollateine alkalinity and methyl orange alkalinity. Water samples were taken for analyses in the lab. A water sample of 250 ml fixed with 1 ml chloroform was taken to derive NO$_3^-$, NO$_2^-$, NH$_4^+$ and PO$_4^{3-}$. To analyse Mn$^{2+}$ and Fe$^{2+}$, a filtered sample of 250 ml fixed with 2 ml HNO$_3$ (65%) was taken. Both samples were contained in glass bottles. A third sample of 250 ml was taken and preserved in PVC bottles to determine Na$^+$, K$^+$, Ca$^{2+}$, Mg$^{2+}$, SO$_4^{2-}$, CO$_3^{2-}$, and HCO$_3^-$. Br$^-$ and Cl$^-$ were determined with samples contained in glass bottles.
Table 5.24 gives an overview of the analyses of different samples. The analyses of the formation water, injection water and the subsequent pumped water are given. For the latter samples the cumulative amount of water pumped up and the time since the start of the ‘pull-phase’ of the tests is given also as reference. Figure 5.48 gives the pH, redox potential Eh and electrical conductivity EC in function of the ratio extracted volume Q over injected volume $Q_{\text{inj}}$. The Eh of the formation water and injection water is positive because these waters were saturated with oxygen. This is also evident from their $O_2$ concentrations. For comparison, oxygen content of water in contact with the atmosphere is 8.26 mg/l at 25°C and 12.8 mg/l at 5°C. During the first part of the test (until 50% of the injected water is recovered) Eh decreases. Then, until all of the injected water is recovered the Eh increases to decrease again afterwards. The increase in Eh is correlated with an increase in oxygen concentration. The EC is more or less constant until 50% of the injected volume is pumped up. Afterwards, the EC decreases continuously until the end of the test. This EC is a reflection of the TDS in the samples. The TDS follows a similar trend. The pH remains more or less constant (7.4) until about 70% of the injected water was recovered. Afterwards, pH decreases towards 6.7 in the last sample.

![Figure 5.48](image)

**Figure 5.48** Evolution of EC, pH and Eh during the push-pull test. $Q/Q_{\text{inj}}$ is the volume of water that was pumped up since the start of the ‘pull-phase’ over the volume of water that was injected.

To see if cations and anions react, the enrichment or depletion of them are calculated in function of the $Q/Q_{\text{inj}}$. The following concentration was calculated for every sample:

$$A_x = X - X_{\text{ref}}$$

where $A_x$ is the depletion (negative) or enrichment (positive) of a cation/anion (mmol/l), $X$ is the concentration of the cation/anion (mmol/l) and $X_{\text{ref}}$ is the concentration in a reference solution of the cation/anion (mmol/l). This reference solution can be the formation water or the injected water. This was calculated for all water samples and is given in figure 5.49.
Table 5.24 Analyses of water samples. Electrical conductivity is given by 25°C. All concentrations are in mg/l. The volume is the cumulative amount of water that is extracted from the well since the start of the ‘pull-phase’ of the test. Nitrate (NO$_3^-$) and carbonate (CO$_3^{2-}$) were below the detection limit in all samples.

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>Volume (l)</th>
<th>Eh (mV)</th>
<th>EC (µS/cm)</th>
<th>O$_2$</th>
<th>Na$^+$</th>
<th>K$^+$</th>
<th>Ca$^{2+}$</th>
<th>Mg$^{2+}$</th>
<th>Fe$^{2+}$</th>
<th>Mn$^{2+}$</th>
<th>NH$_4^+$</th>
<th>Cl$^-$</th>
<th>SO$_4^{2-}$</th>
<th>NO$_3^-$</th>
<th>HCO$_3^-$</th>
<th>PO$_4^{3-}$</th>
<th>Br$^-$</th>
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<td>Pris. Water / 6.6 61 4240</td>
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<td>1 1082</td>
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<td>Inj. Water / 6.8 63 4810</td>
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</table>
Figure 5.49 Enrichment (positive) or depletion (negative) of the pumped water in comparison with the injected water (A and B) and the formation water (C and D). All concentrations are in mmol/l.
Aerobic respiration is the most obvious reaction seen in the analyses. A reductive environment is present in the aquifer, an Eh of −51 mV was measured as the background aquifer value and an Eh of −126 was measured in the above laying peat layer (Vandenbohede, 1998). Oxygen and nitrate are both important oxidants. Oxygenated water that enters an aquifer rich in organic matter will first be freed from its oxygen content and then from its nitrate content. This is apparent on figure 5.49. Oxygen is consumed (figure 5.49A) and its content diminishes sharply to very low values during the first part of the test. Afterwards there is a continuing decrease until about 80% of the injection water is recovered and the dissolved oxygen content is on its background level (figure 5.49C). This oxygen is most likely consumed by organic matter that is present in the sediments:

\[
CH_2O + O_2 \rightarrow CO_2 + H_2O
\]

The extent to which this reaction takes place depends strongly on the reactivity of the available organic matter. Peats for instance or peat fragments in sediments are highly reactive. An important consequence of the above reaction is that CO₂ production within the aquifer may induce carbonate mineral dissolution (Thorstenson et al. 1979; Chapelle et al. 1987).

When most of the oxygen is consumed (from about 80% of the injected volume recovered) the nitrate concentration decreases towards background levels. Before that point no nitrate is consumed in comparison with the injected concentration (figure 5.49A) and the excess concentration of nitrate in comparison with the formation water remains constant. The nitrate is most likely consumed by organic matter present in the sediments. This process is bacterially catalysed and can be written as an overall reaction:

\[
5CH_2O + 4NO_3^- \rightarrow 2N_2 + 4HCO_3^- + CO_2 + 3H_2O
\]

Intermediates of nitrate reduction, like nitrite, are sometimes found in groundwater in low concentrations and are then good indicators for ongoing nitrate reduction, but the process predominantly proceeds to the final product N₂. In this case here, no increase of nitrite concentration was detected. Bacterial nitrate reduction to ammonia is also well know in microbiology (e.g. Zehnder, 1988) and was shown to be of some importance in aquifers (Smith et al., 1991) but the dominant product of nitrate reduction appears to be N₂. From the test results, a very small increase of ammonia concentration is deduced but it may be questionable if it is the result of nitrate reduction or of sampling and/or analyses artefact.

First-order reaction rate coefficients are calculated for aerobic respiration and denitrification according to the method proposed by Haggerty et al. (1998) (see 4.5.2). For the aerobic respiration the observation until 5.5 hours after the start of the test are used (10 observations). Afterwards denitrification takes over. Denitrification first-order reaction rate coefficients are determined on samples taken from 6 hours after the start of the test onward (6 observations). 90%, 95% and 99% confidence intervals are calculated using simple regression. This was not done by Haggerty et al (1998), so these authors had no idea of the accuracy with which they derived their first-order reaction rate coefficients. Results are shown in figure 5.50 and table 5.25.
Figure 5.50 Observations, best fit and confidence intervals of the calculation of the first-order reaction rate coefficients for aerobic respiration and denitrification following the method of Haggerty et al. (1998).

Table 5.25 First-order reaction rate coefficients for aerobic respiration, denitrification and emergence of bicarbonate determined with the push-pull test on the Houtave test site.

<table>
<thead>
<tr>
<th></th>
<th>k (h^{-1})</th>
<th>99% conf. interv.</th>
<th>95% conf. interv.</th>
<th>90% conf. interv.</th>
</tr>
</thead>
<tbody>
<tr>
<td>aerobic resp.</td>
<td>-0.368</td>
<td>± 0.176</td>
<td>± 0.121</td>
<td>± 0.097</td>
</tr>
<tr>
<td>denitrification</td>
<td>-0.731</td>
<td>± 0.349</td>
<td>± 0.211</td>
<td>± 0.162</td>
</tr>
<tr>
<td>bicarbonate</td>
<td>0.411</td>
<td>± 0.527</td>
<td>± 0.318</td>
<td>± 0.244</td>
</tr>
</tbody>
</table>

The aerobic respiration rate is half that of the denitrification rate. Due to the relatively limited amount of observation points the confidence intervals are rather large. How do these figures compare to other test sites? Haggerty et al. (1998) describe a test carried out in an unconfined alluvial aquifer in western Oregon. The site is heavily contaminated by accidental releases of gasoline and diesel fuels at the land surface. The leaking fuels contaminated the unsaturated zone and aquifer to a depth of approximately 5m, resulting in increasing subsurface microbial activity creating widespread anaerobic conditions. Two push-pull tests to measure the denitrification rate resulted in a k of 0.259 h^{-1} and 0.288 h^{-1}. This is in the same extent of our result. However, no indication of the reliability of these coefficients is given.

One of the products of denitrification is bicarbonate. Besides one, probably little erroneous measurement, the amount of bicarbonate remains constant before 80% of the injected volume is pumped up (figure 5.49B). Afterwards this concentration increases. This increase is correlated with the decrease of nitrate and a small increase in pH. The more nitrate is consumed the larger is the enrichment of bicarbonate in the samples. When the nitrate concentration reaches its background concentration the enrichment of bicarbonate in the samples diminishes. Indication that this hypothesis is justified can be found in the calculation of the rate at which bicarbonate is formed. A first-order reaction rate coefficient of 0.411 is found for the appearance of bicarbonate (table 5.25). This value is more or less the same as the rate in which nitrate is reduced taking into account the large confidence intervals of the bicarbonate formation.

Calcium and magnesium concentrations increase slightly during the denitrification process. Calcium and/or magnesium carbonate dissolution might happen due to the increase in bicarbonate. If so, it is only a reaction of minor importance here because the absolute amounts are very small.

It is quite difficult to say something decisively about potassium and sodium based on figure 5.49. Potassium concentrations are decreasing during the latter part of the test as do the sodium concentrations.
Finally some calculations with TRACER3D are performed. This was done to see if the model could cope with flow directly adherent to the pumping well and to see if the above stated explanations could be confirmed by modelling. Due to the symmetry of the problem a two dimensional calculation is performed. The same model as for the injection phase of the forced gradient tracer test on the Houtave test site is used here, so the reader is referred to section 5.2.5 for further details. After the injection phase, the tracer solution is pulled towards the pumping well and the concentration of a number of cations and anions is calculated in the well. This is done by taking the mean concentration of all particles which are present less than 20 cm from the axis of the well at the end of the timestep. These particles are removed from the calculations for the next time step. There are 30 time steps each with a duration of 20 minutes. A new calculation is performed for every anion/cation.

![Figure 5.51](image_url) Comparison between observations and calculated breakthrough curves.

The results of the calculations with TRACER3D are presented in figure 5.51. Breakthrough curve for bromide is calculated first since this is a conservative element and thus a benchmark for further modelling. A good fit between observations (points) and calculation (full line) is obtained from the first run of the model. Therefore, only advective transport is taken into account. The scale of the test is too small on this test site to have important dispersive transport. This was already pointed out with the forced gradient tracer test.

Two calculations are shown for dissolved oxygen. First, tracer breakthrough was calculated without any reactions. This resulted in concentrations that are too high. A first-order reaction rate coefficient of 0.625 h\(^{-1}\) was used to fit the observations. This coefficient is slightly larger than the one derived with
the method of Haggerty et al. (1998) but one has to take also into account the rather large confidence intervals of the latter method. So the model confirms aerobic respiration albeit at a slightly quicker rate.

Denitrification is also confirmed by the model. The simulated concentrations are too large after all the dissolved oxygen is consumed. Denitrification starts from the moment the dissolved oxygen is consumed. The observations are fitted by the same first-order reaction rate coefficient as was derived following the method of Haggerty et al. (1998).

Sodium and potassium concentrations are fitted without taking into account any chemical reaction. This was not clear from figure 5.49. Note that the sodium concentrations of samples taken during the last part of the test are spread largely.

5.7 Discussion and conclusions of the field tests

5.7.1 Forced gradient tracer test

Hydraulic and solute transport parameters were derived on three different field sites. Therefore, the concept of a forced gradient tracer test was put to practice. In all cases, the tests were performed in two steps: first a pumping test and afterwards a tracer test. This resulted in two data sets, observations of drawdowns and concentrations. These were interpreted together to enhance parameter identification. Drawdowns were interpreted with the program package HYPARIDEN, providing a generalised interpretation method for single and multiple pumping tests. A new program package, TRACER3D, was developed for the interpretation of the tracer tests.

The Houtave test site was used as an exploratory case for the concept of the test and the interpretation method. It showed clearly that a forced gradient tracer test could be interpreted with the proposed methodology and the benefits of the test were shown with sensitivity analyses. The design of a double forced gradient tracer test on the Zevergem test site showed clearly that influences of heterogeneity on flow and solute transport can be studied with the test. Finally, a third test was made on the Tessenderlo test site in the framework of design for a remediation technology, showing the direct applicability of the test’s results. Applicability of the parameter identification test will be further discussed in chapter 7. To conclude, two important results of the tests must be highlighted.

A first result is that concentration and drawdown data can be interpreted together and that this results in coherently derived parameters. Otherwise stated, interpretation of pumping and tracer tests can lead to the same parameter values. This has been questioned seriously in literature (e.g. Niemann & Rovey, 2000). Obstacle seems to be the interpretation of the pumping tests. In most cases, interpretation methods based on analytical models are used. These have stringent boundary conditions and oversimplified reservoir schematisations which are not countered in nature. Hence, interpretation methods based on models with much more flexible boundary conditions and reservoir schematisation should be used. The Houtave test site clearly showed that leakage is a very important parameter. Leakage is, however, severely underestimated with analytical models resulting in an overestimation of horizontal hydraulic conductivity of the pumped layer. This was illustrated by calculating tracer breakthrough curves on the Houtave test site based on pumping test interpretation with some analytical interpretation methods. The influence of leakage is highlighted because this test site is characterised by predominantly layered heterogeneity. Lateral heterogeneity is of minor importance. Layered heterogeneity can be built in the reservoir schematisation the applied numerical model. The observed drawdowns can be simulated at any distance to the pumping well, at any level and after every time since the start of the pumping. These properties facilitate the study of layered heterogeneity. The permeable layer on the Houtave test site fore instance was subdivided in two layers from which the individual hydraulic conductivity was derived. If a mean conductivity of this layer would be derived and afterwards solute transport with this value would be calculated, then this would deviate
considerably from the observations. Coherent results of pumping and tracer tests in layered heterogeneous media can thus only be obtained if the leakage is accurately evaluated. Large discrepancies are otherwise possible. One of these cases is illustrated by Niemann and Rovey (2000), who find that the horizontal conductivity derived with a pumping test is 10 to 20 times larger than derived with tracer tests. These pumping tests were interpreted with the Jacob semilog plot of time-drawdown data and with Theis type curve matching. Both interpretation methods are based on the Theis model in which the leakage is completely ignored. Besides the arguments of Niemann and Rovey (2000) concerning the influence of heterogeneity, ignorance of the leakage will thus explain the discrepancy between their pumping and tracer test data.

Obviously, leakage does not explain completely the discrepancies between pumping and tracer tests, especially on field sites where lateral heterogeneity is important. On the Zevergem and Tessenderlo test sites, vertical heterogeneity is by far more important than lateral heterogeneity, but the influence of the latter can not be ignored. In mainly layered heterogeneous groundwater reservoirs, like for instance the Zoutave test site, correct estimation and modelling of leakage is a crucial step. In groundwater reservoirs were lateral heterogeneity is also important, consideration of this heterogeneity will often be vital too. Conclusions drawn here are complementary to previous studies focussing mainly on lateral heterogeneity in groundwater reservoirs. Rovey (1998) for instance showed with digital simulations the influence of lateral heterogeneity on the measured hydraulic conductivity in function of the scale of tests. Such variations, if important, must be accounted for in simulating transport or generally in a modelling exercise. Another example is the MADE site in Columbus MS (USA) where 3-D heterogeneities are important (Feehley et al., 2000). Practical characterisation of the geometry and the modelling of such heterogeneities is quite a different story. In between mainly layered heterogeneous aquifers and mainly lateral heterogeneous aquifers, a plethora of groundwater reservoirs consisting of layered heterogeneity in which each layer displays lateral heterogeneity exists. In these cases, real flow conditions with good estimates of leakage and influence of lateral heterogeneity must be considered as realistically as possible during the interpretation of aquifer tests. Tracer tests give more detailed information on conductivity on a smaller scale than pumping tests, which could lead to different values derived from both tests. For instance, with a tracer tests variations in hydraulic conductivity in function of depth can be derived. A mean will be derived with a pumping test. During the comparison of both results, it will be crucial to have some idea about the heterogeneity and its importance. The heterogeneity was studied with geophysical borehole measurements.

Geophysical borehole logs (natural gamma logs and electrical conductivity logs) were available on the Zoutave and Zevergem test site. These measurements were maximally integrated into the interpretation of the field tests. Most importantly, they provide together with the drilling description the only information about the sediments. Schematisation of the groundwater reservoir is thus largely based on these logs. This schematisation is for obvious reasons of fundamental importance. No good schematisation or otherwise stated no good conceptual model of the groundwater reservoir means no reliable and practical meaningful model results. Besides information on vertical heterogeneity, borehole logs also provide data on lateral heterogeneity, especially the natural gamma log. These data were used in the interpretation of the tracer movement. It is thus argued here to maximally integrate these soft data sets during the interpretation of aquifer tests and hydrogeological modelling in general.

Numerical models provide also a mean of judging the reliability and accuracy with which parameters can be derived through the analyses of the parameters joint confidence region. It is thus known which parameters can not be derived reliably. Take for instance the Zevergem test site. The hydraulic conductivity of a permeable layer in which the tracer was injected was not derived accurately. If this information about the accuracy is not available and solute transport is calculated with the derived conductivity, some surprises are awaiting. It would then be one shot out of a million if pumping test and tracer test would have the same results. Identification of the knowledge gaps and combined interpretation of tracer and pumping tests is thus the way to go, not the comparison of both tests without integration as is usually done.
Molz et al. (1983) concluded that the vertical variation of the hydraulic conductivity plays a vital role in the dispersion process. Therefore, layered heterogeneity must also be included in the interpretation of tracer test data. Horizons with different hydraulic conductivity will tear a tracer plume apart. If these horizons are modelled as one layer with one value for the hydraulic conductivity, a large dispersivity will be needed to model the observations. Knowledge of the heterogeneity is thus also crucial to study dispersivity values.

Secondly, dispersivity could be studied. All three test sites show the same trend: dispersivity is enlarging with travel length of the tracer due to heterogeneity. This is a well established fact found in literature an already discussed in chapter 2 and 3. Derived dispersivities on the three test sites are plotted together with the database summed up by Gelhar et al. (1994) in figure 5.52. Regression lines calculated by Xu & Eckstein (1995) are also indicated. On the scale of the forced gradient tracer tests, no highly reliable values are available. Our values correspond well with the available observation of intermediate reliability. Note that there is a large difference between different field sites. This is not surprisingly since lithologies and synsedimentary and postsedimentary histories of the field sites are different. Sediment of the Houtave test site are relatively homogeneous and are formed in a tidal flat. The Zevergem test site is composed of relatively heterogeneous river bank deposits of the Schelde. Both are quaternary deposits. Tertiary, relatively heterogeneous sand bank deposits are encountered at the Tessenderlo test site. The larger the dispersivity for a given scale, the more heterogeneous the deposits are and vice versa. If this is true, deposits of the Houtave site are the less heterogeneous and of Zevergem the most. Borehole descriptions and natural gamma logs confirm this. This, however, are rather subjective arguments. A more objective analysis is provided with a variogram.

Variograms\textsuperscript{2} are a very useful tool in the description of spatial structures. Consider for instance N measurements \( z(x_1), z(x_2), \ldots z(x_N) \) of the natural gamma in boreholes. The \( x \) stands for the array of co-ordinates of the points where these measurements were taken. The variogram is the plot of the square difference \( \gamma(h) = \frac{1}{2} \left[ z(x_i) - z(x_j) \right]^2 \) against the separation distance \( h = \|x_i - x_j\| \). A variogram is stationary if for large separation distances \( h \), it reaches constant \( \gamma(h) \). On a variogram, the

---

\textsuperscript{2} Mathematical treatment of variograms can be found in for instance Kitanidis (1997) or Deutsch & Journel (1998).
correlation length is the separation distance at which the sill is obtained. The sill is the value around which the stationary variogram stabilises. The correlation length and sill are characteristics of a sedimentary unit. The correlation length and sill can be the same in all directions. Then, it is said that the unit is statistically isotropic. In the other case, the unit is statistically anisotropic. In reality, the vertical correlation scale is almost always found to be smaller than the horizontal correlation scale.

Variograms were calculated based on the natural gamma logs made in all wells on the Houtave and Zevergem test site (figure 5.53). Natural gamma logs are used because the influence sphere of individual measurements is small, thus spatial variability is less concealed. Variograms are calculated in horizontal and vertical direction. From the Houtave test site, only measurements made in the pervious layer are used. First, a raw variogram is calculated based on the observations: for every pair of observations with separation distance h, \( \gamma(h) \) is calculated. If \( n \) observations are made, \( n(n-1)/2 \) dots on the raw variogram are calculated. Then, an experimental variogram is derived through this scatter plot by dividing the axis of the separation distance axis into consecutive intervals. A mean \( \gamma(h) \) is calculated in each interval. Finally, the experimental variogram is modelled to derive correlation length and sill. The most commonly used variogram model is the spherical model:

\[
\gamma(h) = \begin{cases} 
\frac{3h}{2\alpha} - \frac{h^3}{2\alpha^3} & \text{for } 0 \leq h \leq \alpha \\
\sigma^2 & \text{for } h > \alpha 
\end{cases}
\]

where \( h \) is the separation distance (m), \( \sigma^2 \) is the sill and \( \alpha \) is the correlation length (m). The sill equals the variance \( \sigma^2 \) of the distribution, here the variance of the natural gamma observations. Dots in figure 5.53 are the experimental variogram, the full line is the modelled variogram. Table 5.26 gives the variance and correlation lengths. Some general conclusion can be drawn. The correlation lengths are almost the same on both field sites, the vertical being larger than the horizontal. The variance in the vertical direction is larger than in the horizontal direction. This is in both cases due to layering. The
variance in the vertical direction is on both site almost the same. Variance in the horizontal direction is considerably larger on the Zevergem test site. This is in accordance with more heterogeneous sediments and a larger dispersivity. Further, the experimental variograms oscillate after the sill is reached. This may be due to cyclicity in the sediments linked to underlying geological periodicity and or trends in the layering. Even so, it can be due to a too limited data set.

Table 5.26 Variance $\sigma^2$ and correlation length $\alpha$ of the modelled variograms based on the natural gamma observations on the Houtave and Zevergem test site.

<table>
<thead>
<tr>
<th></th>
<th>$\sigma^2$</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Houtave</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>horizontal</td>
<td>0.4</td>
<td>6.0</td>
</tr>
<tr>
<td>vertical</td>
<td>1.75</td>
<td>1.0</td>
</tr>
<tr>
<td><strong>Zevergem</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>horizontal</td>
<td>0.7</td>
<td>7.0</td>
</tr>
<tr>
<td>vertical</td>
<td>1.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>

5.7.2 Push-pull test

Oxygen saturated water with NaBr and KNO$_3$ as tracer was injected on the Houtave test site in a horizon directly under a peat layer. The goals of the test were to observe aerobic respiration, denitrification and other reactions in-situ. First-order reaction rate coefficients could be determined using a simplified method proposed by Haggerty et al. (1998). Bicarbonate was observed as a product of denitrification. The test was modelled with TRACER3D. These simulations showed the above stated conclusion by modelling.
Chapter 6: Effects of aquifer heterogeneity on pumping tests

Effects of Aquifer Heterogeneity on Pumping Tests

Absolute truth is not relevant and is beyond the realm of science anyway. The question is, can we find a model (theory, hypothesis) that ‘works’? George Abell (1982)

6.1 Introduction

Aquifer heterogeneity affects dispersivity and solute transport as shown in previous chapters. This can be studied in the field with tracer tests. But what about hydraulic conductivity? Does aquifer heterogeneity have an effect on the conductivity values derived with pumping tests? Does the derived conductivity value, in analogy with dispersivity, vary with the scale of the test? Various authors have observed that conductivity is function of measurement scale (e.g. Bradbury & Muldoon, 1990; Sauter, 1991; Rayne, 1993). Usually, conductivity increases with measurement scale up to a point beyond which it is approximately constant over at least several orders of magnitude. Available data suggests that different geological media have characteristic measures of scale effect. The slope of the conductivity increase with scale and range differ. Neuman (1994), Rovey (1994), Rovey & Cherkauer (1995) and Sanchez-Vila et al. (1996) have all linked this scale dependency to heterogeneity. Besides aquifer characteristics, well and test characteristics can come into play. Zlotnik (1994), Hyder & Butler (1995) and Butler et al. (1996) have shown that the observed scale increase could also be an artefact of the test method.

Rovey (1998) has studied the effect of heterogeneity on conductivity with a model simulating slug tests in a fractured double porosity model. He pointed out that on a regional scale, flow is primarily along the high conductivity heterogeneities (the joints). Conductivity measured with large scale tests approaches a weighted arithmetic mean controlled by the higher values within a distribution. At smaller scale, a significant portion of the flow must be across the lower conductivity matrix. Therefore, conductivities are weighted harmonically but this is heavily weighted towards the lower values of the distribution. Additionally, if high conductivity pathways are present parallel with the flow, conductivities should be weighted arithmetically. If high conductivity pathways are present perpendicular to flow, conductivities should be weighted harmonically. If high conductivity pathways are present at an angle to flow, conductivities will be between a harmonic and arithmetic mean. These conclusion can be extend to porous media were high conductive pathways are present.

Different studies thus show that heterogeneities influence the derivation of hydraulic conductivity. But it is not straightforward if a harmonic, arithmetic or geometric mean conductivity is derived. In the reminder of this chapter the influence of heterogeneity on pumping test interpretation is studied in a Theis type of aquifer or otherwise stated in a confined aquifer. To simplify matters, the influence of leakage is thus neglected. Only the influence of heterogeneity in the pumped layer is studied this way. Therefore, pumping tests are simulated in a heterogeneous aquifer with a finite-difference bloc-centred numerical groundwater flow model. Observations are generated with the groundwater flow model and
Chapter 6: Effects of aquifer heterogeneity on pumping tests

interpreted with the inverse pumping test interpretation model of HYPARIDEN, based on an axi-symmetric numerical model. Heterogeneity of the reservoir is compared with the derived conductivity value. Heterogeneous groundwater reservoirs are modelled geostatistically. The influence of scale, number of observations, variance of hydraulic conductivity and correlation length will be studied.

6.2 Groundwater flow model RMOQ3D

6.2.1 General introduction

The groundwater flow model RMOQ3D (Regional Modelling Quasi-3D) (Lebbe, 1978) is used to simulate pumping tests. It is a finite difference model to simulate groundwater flow in porous media very similar to MODFLOW. The model structure resembles the MODFLOW structure, which allows packages to be added (infiltration, wells, rivers, constant head). Steady state as well as unsteady state flow can be calculated. The groundwater reservoir is subdivided in a number of layers, rows and columns. Every grid block has a nodal point. The groundwater reservoir is always bounded below by an imperious boundary and above by the water table. A value for the horizontal hydraulic conductivity and specific elastic storage (for transient flow calculations) is awarded to every node. It is supposed that the hydraulic parameters like the specific elastic storage, the storage coefficient near the water table are constant within the finite-difference cells. The other parameters like the horizontal conductivity and the resistance are supposed to be constant on the boundary plane of the finite-difference cells. The thickness of the uppermost layer is calculated during the successive iterations to reflect water table movements. It is equal to the calculated hydraulic head minus the given level of the base of the uppermost layer. Hydraulic heads are situated in the nodal points of the cells. Two types of boundary conditions can be introduced directly in the finite-difference model. Those are the impervious boundaries and the constant head boundaries. The constant flow boundary condition can be introduced indirectly with the aid of impervious boundaries and discharge or injection rates. The groundwater flow equation is rewritten into a set of finite-difference equations and solved iteratively with alternating direction implicit method (ADI) (Peaceman & Rachford, 1955; Douglas & Peaceman, 1955; Douglas & Rachford, 1956). For this iterative method initial values for the hydraulic head (estimated values for a steady state simulation or results from a steady state simulation for an unsteady state simulation) are introduced together with the reservoir schematisation, hydraulic parameters, boundary conditions and additional packages (infiltration, wells, rivers, constant head). It is supposed that the hydraulic heads of one direction, e.g. a column, are unknown while the surrounding values of the hydraulic heads of the bounding finite-difference cells are known. As many equations as there are unknowns are thus obtained. The set of equations are solved and the calculations are continued for the next column. The ADI-method continues by supposing that the hydraulic heads of another direction (e.g. row) are unknown while the hydraulic heads of the surrounding finite-difference cells are considered to be known. The set of equations are resolved and the calculation is continued for the next row. To conclude the iteration, the same is done for the layers. During one iteration the finite-difference equations are thus solved three times. Heads are then compared with the results from the previous iteration. If the difference is below a certain value (the closing criterion) a solution is reached.

6.2.2 Simulation of pumping tests in a homogeneous aquifer

First, a pumping test is simulated with RMOQ3D. Observations are generated in different observation wells. These observations are interpreted with HYPARIDEN and the hydraulic conductivity of the pervious layer is derived. This was first tested with in a homogeneous aquifer to verify if RMOQ3D could simulate a pumping test accurately. The pumping test is simulated with unsteady state
Chapter 6: Effects of aquifer heterogeneity on pumping tests

A. Vandenbohede

The model area is 240*240 m² large. Cells are 1 by 1 metre so 240 columns and rows are used. Two layers are included, a pervious lower layer (layer 1) with thickness of 10 m and an impervious upper layer (layer 2) with a thickness of 2 m. Horizontal conductivity of the pervious layer is 10.0 m/d and 0.01 m/d for the impervious layer. Specific elastic storage is $0.5 \times 10^{-4}$ m$^{-1}$ for both layers. Bottom of the pervious layer is impervious and the hydraulic resistance between both layers is 999999.9 d. So, layer 1 is confined and the aquifer is a Theis type of aquifer. The storage coefficient near the water table is 0.2. Because of the very large hydraulic resistance between layer 1 and 2 the hydraulic parameters of layer 2 have no influence on the drawdowns in layer 1. Because of the symmetry only one quarter of the depression cone is simulated. The pumping well is situated in the first column, first row and first layer (upper left-hand side cell). Discharge rate is 180 m³/d. The boundaries are all impervious. The simulation time is 43.57 minutes and 13 stress periods are used. The length of the first stress period is 0.72 minutes and every further stress period is $10^{0.1}$ times larger than the previous. Closure criterion is 0.1 mm.

Figure 6.1 shows the contour lines in layer 1. The time-drawdown curves are also given for observation wells at three different distances from the pumped well. Plotted on semi-logarithmic paper the evolution of drawdown with time must be nearly linear if $u<0.01$ (Cooper and Jacob, 1946) where

$$u = \frac{r^2 \cdot S_r}{4 \cdot K_h \cdot t}$$  \hspace{1cm} (6.1)

$t$ is time (d) since the start of the pumpage and $r$ is the distance (m) between the observation and pumping well. These conditions ($u<0.01$) are not fulfilled in the case of small times and large distances. It explains why there is a small deviation from a straight line for an observation well placed at 19.7 m from the pumping well just after the start of the pumping.

![Figure 6.1](image)

*Figure 6.1* Drawdown contour lines in layer 1 for a homogeneous aquifer (scale in metre). Inset shows the evolution of drawdown in function of time for three observation wells placed at 5.6, 12.7 and 19.7 meter from the pumping well.
Boundary conditions can be a factor of error. Drawdowns propagate as a wave away from the pumping well. This wave is reflected when it reaches the model boundaries, interfering with the calculations closer to the pumping well. Therefore, the duration of the pumping test is only 43.57 minutes long. The reflection is then minimal and the errors on the calculated observations are small.

Observations were generated in three wells located at a distance of 2.12, 6.36 and 12.02 m from the pumping well. These were interpreted with the inverse numerical model of the HYPARIDEN programme package. The same discretisation and parameterisation as in the RMOQ3D model is used. Derived value for the horizontal conductivity of layer 1 is 10.56 m/d and $0.54 \times 10^{-4}$ m$^{-1}$ for the specific elastic storage. This means that RMOQ3D is capable of simulating accurately a pumping test within the considered short time span.

![Conductivity field](image)

**Figure 6.2** The conductivity field for four different combinations of the sill c and correlation length α. Horizontal and vertical axis are distances given in metre.

**6.2.3 Simulation of pumping tests in a heterogeneous aquifer**

It has been stated in chapter 2 and 4 that average conductivities of for instance a layer are derived with pumping tests. The aim of this part of the study is to look at the influence of aquifer heterogeneity on pumping test analyses and more specifically on the conductivity value which is derived in a Theis type
of aquifer. The schematisation presented in section 6.2.1 is used but every grid block is appointed a different conductivity value. The pervious layer is not further subdivided in more layers and every grid block is 1*1*10 m. This means basically that the influence of lateral heterogeneity is studied in a two dimensional aquifer.

A sequential gaussian simulation procedure (Deutsch & Journal, 1998) is used to generate heterogeneous hydraulic conductivity fields, by assuming that ln(k) is a random function characterised by a spherical variogram γ:

\[
\gamma(h) = \begin{cases} 
\frac{3h}{2\alpha} - \frac{h^3}{2\alpha^3} & \text{for } 0 \leq h \leq \alpha \\
\sigma^2_{\ln(K)} & \text{for } h > \alpha
\end{cases}
\]

where \( h \) is the separation distance (m); \( c \) is the sill, which is equal to the variance on ln(K) \( (\sigma^2_{\ln(K)}) \) and \( \alpha \) is the correlation length (m). The average of the ln(K) distribution is 10.0 m/d. Correlation length and variance of ln(K) are varied to see what the influence of both parameters is on the pumping test interpretation. Two different correlation lengths (0.5 and 25 m) and six variance of ln(K) (0.01, 0.1, 0.5, 1.0, 2.0 and 5.0) are considered, resulting in 12 different combinations. Figure 6.2 illustrates the conductivity field for a number of different situations focussed on a square of 10*10 m. This is the scale on which the observations will be made. Small variances and correlation lengths lead to a geometrically quick varying conductivity field. The same can be said of the combination small variance and large correlation lengths but the distances between zones of large conductivity are now larger. Small correlation lengths and large variance shows a geometrically quick varying conductivity field with locally very large values. Large variances and large correlation lengths result in a gently varying conductivity field. The particular field shown in figure 6.2 has relatively small conductivity values enlarging to the right-hand side corner. The side of the region is 2.5 times smaller than the correlation length.

Ten realisations were made for every correlation length and standard deviation. One pumping test was simulated in with every realisation and interpreted using HYPARIDEN. Observations are generated in three observations wells, respectively at a distance of 2.12, 6.36 and 12.02 m from the pumping well. The observations of all three wells are interpreted simultaneously. Observations made in one well were also analysed but only for one realisation of the conductivity field. The results are presented in figure 6.3. Derived conductivity, marginal standard deviation and sum of the squared residuals is shown in function of the variance on ln(K) for the two different correlation lengths. Some interesting conclusion can be drawn from these figures:

- If the variance on ln(K) is relatively small (less then 0.1 to 0.3), the derived conductivity value equals or is very close to the average aquifer conductivity. This means that with pumping tests, the average hydraulic conductivity will be derived in moderately heterogeneous aquifers.
- With a correlation length of 0.5 m, the derived conductivity increases in function of c which is the variance on ln(K) meaning that the derived value is strongly influenced by the high conductivities in the generated conductivity field. Due to the small correlation length, highly conductive pathways come into existence. The difference between derived values from different realisations becomes larger with c. Thus, in heterogeneous aquifers pumping test performed on different locations do not necessarily result in the same conductivity value. Notice that in the case of a highly heterogeneous aquifer, the arithmetic mean of different pumping tests does not equals the aquifer’s arithmetic mean conductivity. The situation is different for the case where the correlation length is 25.0 m. Different realisations with large standard deviations results in a large interval of derived conductivities, both small and large values are found. This is because the scale of observation is smaller than the correlation length. In one realisation, the pumping and observation wells are situated in a zone with small conductivities or in a zone with large conductivities or in a transitional zone. Important is that when different pumping tests are performed in the same aquifer.
but on different locations the arithmetic mean of the inferred conductivity equals the arithmetic mean aquifer conductivity.

**Figure 6.3** Derived conductivity, marginal standard deviation and sum of the squared residuals in function of the variance on ln($K_h$) for two different correlation lengths. Results are given if drawdowns from three observation wells are used and if drawdowns from only one observation well are used. In the latter case, two different distances (2.12 and 12.02 m) from the pumping well are considered.

- The marginal standard deviation and sum of the squared residuals increase with c. The accuracy and reliability with which parameters are derived is thus weaker in the case of a heterogeneous aquifer.
- The conclusions concerning the derived conductivity with three observation wells are also valid using only one observation well. The marginal standard deviations and sums of squared residuals, however, do not increase significantly with c as was the case with three observation wells. Using
one observation well, one gets the impression that the conductivities are derived relatively reliable and accurate. They can, however, differ considerably from the derived value using three observation wells. It is thus preferred to use more than one observation well. The drawdown in an observation well is a function of the conductivity between the pumping and observation well. If only one observation well is present, the observed time-drawdown curve can easily be fitted. Because the difference between the observed and the calculated drawdowns is very small, one obtains small sums of the squared residuals. Consequently one gets the false impression that the horizontal is accurately inferred. The derived conductivity will be a average value of the ones present between pumping and observation well and can vary considerably depending on the location of the observation well. Thus no average aquifer value is derived. No indication of possible influence of aquifer heterogeneity is obtained. If there are two or three observation wells, it is by far more difficult to match the all time-drawdown curves nicely. The derived conductivity will be an average value of the ones present between pumping and the most distant observation well but the marginal standard deviation and sum of squared residuals will be large. These large parameters give thus an indication that the aquifer is quite heterogeneous. This is illustrated with an example in figure 6.4. It shows that the drawdowns of one observation well can be simulated flawlessly whereas significant differences occur between the calculations and observations using three observation wells.

Figure 6.4 Time-drawdown curves of a pumping well performed in a heterogeneous aquifer with correlation length of 0.5 m and a variance of $\ln(K_h)$ of 5.0. The data of three observation wells were interpreted simultaneously or only data obtained in one observation well were used (located at 2.12 or 12.02 metre from the pumping well). Crosses are the observations and the full lines are drawdown calculated with the optimal parameter values. The table shows the derived conductivity $K_h$, marginal standard deviation $s_m$ and sum of squared residuals $A$. 

![Graph showing time-drawdown curves](image)
6.3 Field example

Two observation wells placed at the same distance from the pumping well but in different directions should show more or less the same drawdowns in function of time in a homogeneous aquifer. This is not the case in a heterogeneous aquifer. Data from the Zevergem test site illustrates this. IP1 and IP2 (see figure 5.23) are placed both at 7,5 m from the pumping well but 180° apart. PB2 is found 2,5 m from the pumping well between PP and IP1. PB3 is also located 2,5 m from the pumping well but between PP and IP2. Figure 6.5 shows the drawdowns measured in these wells during the pumping test described in section 5.3.3.

IP1 and IP2 are situated in layer B, a moderate to coarse sand. It has a horizontal hydraulic conductivity of 24 m/d between IP1 and PP. Hydraulic conductivity between IP2 and PP is smaller, 9 m/d. Measured drawdowns in IP1 and IP2 do not differ much, only 2 to 3 cm. This small difference is related to the relatively large distance from the pumping well. The drawdown measurements in these wells are influenced by the average hydraulic conductivity of sediments between the observation and pumping well, thus by a relatively large aquifer volume. Hence the drawdowns are more or less the same.

PB2 and PB3 are situated in layer A, which consists of alternating clay and siltous sand layers. Drawdowns in these two wells differ about 7 to 8 cm, the largest drawdown is measured in PB2. The wells are placed below a more clayey layer as can be seen on the natural gamma logs (figure 5.24). PB3 is also located in slightly more clayey sediments than PB3. It is quite impossible to indicate the exact reason of the difference. Local differences in hydraulic conductivity, hydraulic resistance and a combination of both are possible.

![Figure 6.5](image_url)

**Figure 6.5** Drawdowns measured in observation wells IP1, IP2, PB2 and PB3 on the Zevergem test site (upper figure) and the difference between drawdowns measured in IP1 and IP2 (IP1 minus IP2) and PB2 and PB3 (PB2 minus PB3) (lower figure).
Albeit, the noteworthy drawdown differences between wells placed at the same distance of the pumping well but in different directions indicates together with the borehole logs and the results from the tracer test the heterogeneity of the field site.

In most cases, no wells will be drilled at the same distance from the pumping well because they theoretically provide the same information. Comparison between observations and drawdowns calculated with the derived optimal parameter values are also interesting as was indicated in figure 6.4. With different observation wells available, a qualitative indication can be obtained about aquifer heterogeneity. In heterogeneous aquifers, drawdown measurements in one or more observation wells will deviate importantly from the drawdowns calculated with the derived optimal parameter values.
Chapter 7

Applications of field derived parameters

Models as a synthesis of available knowledge

Models are to be used, but not to be believed. (Henri Theil)

7.1 Introduction

Different parameter identification tests are available in hydrogeological research and many different parameters can be determined. But what to do with them? How can the knowledge of these parameters be implemented to solve practical issues, how can they be useful to the practitioner in the field? That is the theme of this chapter.

A distinction is made in two types of applications. The first type of application is on a scale that is approximately the same as the one on which the parameters are derived: for instance in situ clean up and remediation of field sites. Parameter tests deriving necessary parameters are designed on the same scale as the remediation technology. Secondly, the scale of application is larger than the scale of the test: regional groundwater flow and solute transport models. An important question is then how to translate locally derived parameters in these models, considering the fact that aquifers are heterogeneous.

7.2 Field scale applications

7.2.1 Introduction

The final go ahead of the remediation of a contaminated site should just be the end of an intense investigation and decision making process. Remediation of contaminated sites is costly. Different alternatives should have been taken into consideration on a scientific, practicable and financial basis. In addition, the problems encountered in remediation need quantitative answers. Therefore, reliable values of parameters describing the groundwater reservoir and the remediation scheme must be known, hence the importance of reliable tests to derive these values.

Hydrogeological site investigation is an important first step in this process. The purpose of this site investigation is to characterise soil and groundwater pollution problems in sufficient detail to facilitate the design of a cost effective corrective action program. It entails actual measurements of the physical and chemical processes that control the contaminant transport at the given site. Hydrogeological site investigation is in this context a procedure in which three types of data should be collected. First, relevant geological data of the site should be collected. Sedimentological relevant data should be gathered and a stratigraphic profile must be made. Secondly, a hydrogeological data are to be
collected. Hydraulic head and relevant parameters are to be determined. Thirdly, there is the chemical data. Water samples should be collected and analysed to map the extent of the contamination. It is obvious that these data are collected simultaneously and are integrated to define the nature and extent of the contamination as well as the potential migration of these contaminants within the natural groundwater systems. After the delineation of the problem and the estimation of the potential future hazards, a remediation scheme can be designed. Parameter identification tests come into play an all these steps. For instance, pumping tests, tracer tests or a combination of both, allow the determination of the necessary hydraulic and solute transport parameters. Chemical reactions can be studied and quantified with specific tests, for instance push-pull tests. It is of considerable advantage that in many cases these tests are on the same scale as the applications.

Once a site has been characterised, control and remediation options can be selected to provide an overall clean up strategy. Choosing a remedial technology is a function of contaminant type, site hydrogeology, source characteristics, location and distribution of the contaminant and available technology. In most cases, there will also be financial restrictions. The use of parameter identification tests in the process is illustrated with a case study of a site contaminated with 1,2-dichloroethane.

7.2.2 Case study: Tessenderlo test site.

7.2.2.1 Introduction

The case study of a site contaminated with 1,2-dichloroethane (1,2-DCA) is situated in Tessenderlo. 1,2-DCA is a saturated chlorinated aliphatic hydrocarbon, a group containing also chloroethanes, -propanes and –butanes. In industry they are mainly used as degreasing agents, detergent, paint removers, solvents and chemical intermediates in the production of a whole range of products. Chlorinated ethanes can be used as intermediates for the production of chloroethenes, explosives, dyes, and in rubber vulcanizing processes. Especially 1,1,1-trichloro- and 1,2-dichloroethane are produced in large quantities. Chlorinated C$_2$ to C$_4$ alkanes occupy the top rankings of the American and European priority lists (Hughes et al. 1994) for clean up. Most of the worldwide contamination results from accidental leakage during production, application or transport.

Its (bio)degradation in the environment is very slow (half-life time of about 50 years) under reductive conditions. It is a possible health hazard (cancerogenic) since 1,2-DCA is oxidised to chloroacetyldehyde. The maximum admissible concentration in groundwater is 30 µg/l (Vogel et al., 1987). No in situ detoxification technology with an application to groundwater is available. A new bacteria, Desulfitobacterium dichloroeliminans strain DCA1, was identified at the Laboratory for Microbial Ecology and Technology (LabMET) of Ghent University that can detoxify 1,2-DCA quickly in anaerobic circumstances and without producing other hazardous products (De Wildeman, 2002). This new technology was to be used in an in situ application. In the presence of a low-cost C/N/P source, pH of 6-8 and reductive circumstances this technology can be successful. Different design options for remediation were open for discussion. One option is the design of a bacterial screen through which the groundwater flows. Another is a pump and treat system.

The decision making which remediation will be chosen is not the issue here. Preliminary discussion can be found in Linthout (2003). Here, it is shown how parameter identification tests can be integrated in this process. To come to a feasible in situ remediation with strain DCA1, some basic questions must be answered:

- Fundamental knowledge about hydraulic and solute transport properties of the field site should be collected. Particularly hydraulic conductivity, porosity and dispersivity are of interest. They determine advective and dispersive transport and thus the spread of solute in the aquifer. Therefore, a pumping test and a tracer test were performed.
• Activity of strain DCA1 was proven in the lab. This has to be extended to a field situation. Therefore, a push-pull test was performed to demonstrate the detoxification activity of strain DCA1 under field conditions.

• It is not known if strain DCA1 is mobile in porous media. If yes, possible retardation of it should be known. Therefore, a transport test in which strain DCA1 is injected in one well and is pulled towards a second well, was performed.

7.2.2.2 Towards a remediation scheme

The characteristics of strain DCA1 to detoxify 1,2-DCA were first investigated intensively in the lab (De Wildeman, 2002; Linthout, 2003). At 13° C, the groundwater temperature, and pH 6.8 the 1,2-DCA concentration in the groundwater samples (50 ml) dropped below the detection limit (0.1 mg/l) within 12 days after inoculation. The activity of strain DCA1 was also shown in contaminated groundwater ex situ on larger scale (1000 l) (Linthout, 2003). Then tests were made to prove the activity of strain DCA1 in situ.

First, a step-drawdown test and a forced gradient tracer test were performed. The results of these tests provided knowledge of the hydraulic and solute transport properties of the aquifer as described in section 5.4. These results were used to design further tests. Since the forced gradient test was performed on the same scale as further tests and of the ultimate remediation scheme, important issues could be answered. Suspected drawdowns in function of discharge rate could be predicted, travel times and residence times for conservative constituents could be calculated and dispersive properties were known. The latter is very important issue to know in the case a solute with for instance strain DCA1 or a carbon source is injected in the groundwater reservoir. Relevant question is then how the transport (advective and dispersive transport) of 1,2-DCA and a carbon source will be.

The activity of strain DCA1 must be shown in situ. Therefore, a push-pull test was performed. The test is fully described by Linthout (2003). Water was extracted from LV52 with a discharge rate of 2m³/h during 45 minutes and injected in LV22B (figure 5.36). Together with this water strain DCA1, NaHCO3-buffer and a yeast extract were dosed in the anaerobic injection water. The buffer maintains a favourable pH in the injection water. Yeast extract was added because laboratory experiments showed that it has a positive effect on the dechlorination rate. In all, 1.5 m³ of contaminated groundwater and 70 l inoculum were injected. No conservative tracer was, however, added. This was done to make the preparation of the injection water not too complicated and because the tracer constituent might influence DCA1 activity. The test had a duration of 36 days, water samples were taken daily or every two days. Discharge rate was not constant during the test’s duration.

The absence of a conservative tracer and the non-constant discharge rate hinder the interpretation of the test and derivation of a first-order reaction rate coefficient. It was seen that 1,2-DCA concentrations were declining rapidly, becoming almost below the detection limit after pumping up 113.3 l. This is only 7.6% of the volume of injected water. Fortunately, the discharge rate during the first 8 days of the test was more or less constant, being 0.045 m³/d. Now, with some basic assumptions an estimate of a first-order reaction rate coefficient following the method of Haggerty et al. (1998) can be made. Assumptions are that the discharge rate during the first 8 days is constant and that the relative concentration of a fictive added conservative tracer would be 1 during this period. First-order reaction rate coefficient for the detoxification of 1,2-DCA is then calculated according to Haggerty et al. (1998). Results are given in table 7.1 and the regression line is shown in figure 7.1.

<table>
<thead>
<tr>
<th>$k$ (d$^{-1}$)</th>
<th>95% conf. interv.</th>
<th>90% conf. interv.</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.592</td>
<td>± 0.427</td>
<td>± 0.338</td>
</tr>
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Table 7.1 First-order reaction rate coefficient with its confidence intervals for the detoxification of 1,2-DCA by strain DCA1.
First-order reaction rate coefficient is $-0.592 \text{ d}^{-1}$. This means that the 1,2-DCA concentration is reduced to 50\% in 1.17 days, to 25\% in 2.34 days and to 10\% in 3.89 days. For comparison, laboratory test at 13°C and addition of yeast and vitamin K2 resulted in a half-live time of 9.64 days which is considerable slower than the field value. Notice, however, the relatively large confidence intervals of the derived field value. In addition, quality of the inoculum, pH, eH, additive, etc all have their influences on the detoxification process and half-live times as was found in the laboratory (Linthout, 2003).

Important result of the push-pull test was, however, that it clearly showed the detoxification of 1,2-DCA by strain DCA1 in situ. The first-order reaction rate coefficient could be approximated, keeping in mind the assumption which must be made (discharge rate was simplified as being constant and the relative concentration of a fictive conservative tracer was 1). This is an important constant to know since it describes the time that is needed to detoxify 1,2-DCA. This time must be known in the design of a future remediation.

![Figure 7.1 Observations, best fit and confidence intervals of the calculation of the first-order reaction rate coefficients following the method of Haggerty et al. (1998).](image)

Then the mobility of strain DCA1 in the porous medium was investigated. Therefore, a transport test was performed (Linthout, 2003). Water was pumped from LV52, lactate (as carbon source), strain DCA1, bicarbonate (as buffer) and yeast was injected in LV22B. In all, 1.2 m$^3$ of water was injected. Groundwater with lactate was also injected in LV22A and LV51, respectively 2 and 3 m$^3$. This was done to create a zone with a carbon source between injection well LV22B and pumping well LV52. Until 14 days after the injection, 1,2-DCA concentration was followed in LV22B. No pumping occurred during this period. The 1,2-DCA concentration decreased to under 1 mg/l. Then pumping started on LV52. The 1,2-DCA concentration increased temporarily slightly in LV22B but decreased then back below 10 mg/l for the remainder of the test. This means that water that flows through the bacterial zone created around LV22B and contaminated with 1,2-DCA is treated. This was the case even after 100 days of pumping on LV52. Aim of the test was, however, to see if strain DCA1 is mobile in the groundwater reservoir. No clear indications for that can be found. The fact that 1,2-DCA concentrations are very low in LV22B means that it is detoxified by strain DCA1 around LV22B. The bacteria thus stay around LV22B more than 100 days despite the pumping on LV52. 1,2-DCA concentrations decreased very slowly in LV51 indicating only minor presence if all of strain DCA1 around this observation well. The decrease is most probably due to mixing of treated water that flowed through the bacterial zone around LV22B and water that bypassed it.

The presence of strain DCA1 in different samples was studied. Therefore, DNA of the microbial population present in the samples was multiplied using an universal primer in a PCR-apparatus. DNA
was separated with gel electrophoresis. Strain DCA1 could not be pointed out in samples extracted from LV51. This was also the case for samples from LV22B. Most likely the applied PCR technique is not sensitive enough using universal primers (Linthout, 2003).

7.2.2.3 Conclusions

Much important work has been done on the Tessenderlo test site. Basic hydraulic and solute transport parameters were derived and in situ activity of strain DCA1 was proven. Indication of the first-order reaction rate coefficient was obtained. Questions, however, remain before a definitive remediation can be started. What for instance is the retardation of strain DCA1 in porous media and in particular in the sediments found in the Tessenderlo test site? Are the bacteria mobile at all? The presence of clay and more particularly of glauconite, whose influences on solute transport (of bacteria, lactate, etc) are not well known, deserves further attention. Some parameters such as 1,2-DCA concentration, pH, eH, are far less controllable in situ than on the lab. How do these fluctuating parameters influence strain DCA1 activity?

7.3 Regional scale applications

7.3.1 Regional groundwater flow models

Hydrogeological models are characterised by the fact that the obligatory input, with its uncertainty, is plenty but the observations are few. The input consists of a conceptual model of the problem and its different kind of parameters. Parameters are divided in physical parameters (hydraulic and solute transport parameters, infiltration, stresses, etc) and model parameters (discretisation, closure criterion, number of particles in case of solute transport, etc). Observations are hydraulic heads, concentrations, stream flows, etc. Parameters can become to a certain extend observations providing they are derived with appropriate tests.

During the process of calibration these conflicting characteristics must be reconciled in the most elegant way. The focus of the discussion here is about the application of field information, field derived parameters as well as other observations in numerical models. For that, some guidelines are available. The most widespread are those summed up by Hill (1998).

A general model protocol or framework is presented in figure 7.2. It must be stressed that each groundwater model is unique and can deviate from this general scheme. The first and a very important step is defining of the goals of the simulations and questions which are to be solved by the modelling. A distinction must be made between descriptive and predictive modelling. The aim of a descriptive model is to describe a groundwater flow system, how it behaves now and how it behaved in the past, quantitatively and/or qualitatively. A predictive model is used to make predictions towards the future. In the first case, historic and/or current observations are available to calibrate the model. This is not the case for a predictive model. It is based on the description of the current situation which is then extrapolated. It is thus highly influenced by the quality of a basic descriptive model.

In a second step, ideally, an initial set of observations is collected specifically for the modelling exercise. These are drillings to define the groundwater reservoir, hydraulic head measurements, water quality analyses, aquifer test analyses, geophysical survey data etc and information found in literature. Based on the previous steps, the available information is summarised in a conceptual model. This conceptual model includes the geometry of the model region, number of layers, columns and rows, boundary conditions, sources and sinks, processes that will be included in the model, etc. The conceptual model must be seen as a synthesis of all available hydro(geo)logic and other relevant data.
and knowledge of the study area. The construction of a conceptual model is a highly important step. Both oversimplification and undersimplification must be avoided. An oversimplified model fails to capture the essential features of the real-world system. On the other hand, an undersimplified conceptual model tends to make it too complex and too computational demanding and relations between different parameters become very obscure. It is practical to build the conceptual model as an ‘open’ architecture. In this way, during the modelling or if more observations become available, the model can be altered or expanded.

The selection of the computer code is based on the aforementioned steps. What are the goals, what is the complication needed, available observations, conceptual model, must solute transport be calculated, density effects...? The conceptual model is then translated into the chosen numerical scheme. Calibration and sensitivity analyses will be discussed more in detail below.

Figure 7.2 A general model protocol (Zheng & Bennet, 2002).

Ideally, a model is an iterative exercise as indicated in figure 7.2. Repeated steps of data gathering or making changes to the conceptual model and calibration will lead to a good end results. Unfortunately, in many instances no time is available to perform more than, at best, a very limited number of iterations.
A model is calibrated by adjusting the input parameters and initial and boundary conditions until the model simulation matches the field observations to a reasonable degree. During this process, sensitivity analyses are used to test the overall responsiveness and sensitivity of the model to certain parameters. Calibration is an inverse problem since field observations are used to derive optimal input parameters.

During model calibration, three important problems can be encountered: non-uniqueness, insensitivity, and instability. Non-uniqueness means that different combinations of parameter values will lead to the same results. Insensitivity occurs when the observations do not contain enough information to derive the parameters; they are insensitive for these parameters. Instability means that minor changes in a parameter value or observations radically change the model results. Non-identifiability of parameters is closely related. The observations do not support the derivation of a certain model parameter. One practical solution to these problems is to collect and use adequate observations, which are sensitive to the parameters of interest. Sensitivity analyses can point to these observations providing the conceptual model represents the field situation well. The use of sensitivity analyses and the calculation of correlations between parameters can identify non-uniqueness. These subjects have been discussed for the development of the forced gradient test (field test in Houtave) but these conclusions are also valid here.

Model calibration is frequently carried out by trial and error, running the forward model repeatedly and manually adjusting the input parameters selected for calibration until the model suits the observations. There are, however, many limitations associated with this method. It is difficult to get in touch with reasons for non-uniqueness, insensitivity, and instability unless countless runs with slightly different parameter values are made. Additionally, there is no guarantee that, at the end, the optimal solution is found. An interesting alternative to remove some of the subjectivity of the trial and error procedure is the use of inverse techniques as was discussed in the section on pumping tests. Several computer codes are available for automated parameter identification in flow modelling. Examples are MODFLOW (Hill, 1992), PEST (Doherty, 1994), UCODE (Poeter & Hill, 1998) and MODFLOW-2000 (Hill et al., 2000). PEST and UCODE can be adapted to utilise concentration data in estimating transport parameters while MODFLOW-2000 can utilise travel time data in flow calibration (Anderman & Hill, 1997). SUTRA (Piggott et al., 1994) is another code for inverse flow and transport modelling. Inverse modelling has some advantages over the traditional trial and error calibration. It provides a consistent framework and objective criteria to systematically evaluate the goodness of fit between model results and field data and quantitatively analyse the sensitivity and uncertainty in estimated parameters. An inverse model procedure and benefits of inverse modelling are discussed and illustrated with the forced gradient tracer tests. This is also valid for larger regional models. Some general aspects of automated model calibration are given in Zheng and Bennet (2002) and guidelines are provided by Hill (1998).

An important difference between HYPARIDEN and a regional groundwater flow model is the model complexity. The pumping test model is ideally suited for inverse modelling due to more straightforward relations between different parameters and between parameters and observations. This is less the case with regional groundwater flow models. Also, more parameters, boundary conditions, external stresses, and so on are present and the lithology on this larger scale is far more varied and only fragmentary known for sure. It is therefore quite difficult to construct a converging inverse regional groundwater flow model. However, techniques and guidelines used with inverse models are very interesting to apply. This is done in the following sections were two density dependent models of groundwater flow and solute transport in the Belgian coastal plain are simulated. The first, in the eastern coastal plain involves the formation of a fresh water lens under an old inverted channel ridge, the second, situated in the western coastal plain, involves the groundwater flow under the sea, shore, dunes and polder area. The goal of the simulations is to visualise the evolution of the distribution of fresh and salt water and to study some factors influencing it. Therefore, no inverse model is made but a forward model is used. However, in the calibration process sensitivity analyses are used and the models are an integration of available field knowledge of the problem.
For the calibration of the two models the already mentioned guidelines of Hill (1998) are used. Although drafted with inverse modelling in mind, many of the guidelines are very constructive for trial and error calibration. These guidelines are given below and discussed with the two case studies in mind.

**Guideline 1: Apply the principle of parsimony**

Or otherwise stated, keep the model as simple as possible but not simpler. A delicate balance between a relatively simple conceptual model and numerical code and a good representation of the systems characteristics for the application must be found. Complexities are also added in a later stage of the modelling so that its influences can be readily discerned.

**Guideline 2: Use a broad range of information to constrain the problem**

The model must respect what is known about the hydro(geo)logy. The modeller should use all available information about the problem to construct the best suited conceptual model and during the calibration, that is drilling description, geophysical measurements, aquifer test results, water quality analyses, sedimentological data, … and of course general (hydro)geological knowledge of the region. A groundwater flow model must thus be seen as a synthesis of all available knowledge relevant for the solution of a certain problem.

**Guideline 3: Maintain a well-posed, comprehensive regression problem**

A well-posed regression problem is one that will converge to an optimal set of parameter values given reasonable starting parameter values. Guideline 3 is intended for inverse modelling. However, some of the concepts of inverse modelling are also used in the case studies. Sensitivity analyses show many characteristics of a model. As illustrated in the section on the forced gradient tracer tests, sensitivity analyses indicate which parameters are sensitive in a certain problem and how one parameter is correlated to the others. Highly correlated parameters can not be identified uniquely. They indicate thus which parameters must be calibrated, via trial and error or via inverse modelling. Additionally, sensitivity analyses show where observations are to be made which have information to derive or calibrate parameters. If a hydraulic conductivity is only sensitive for head measurements in places A, B en C, these are the places were the observations must be made. Thus sensitivity analyses are very helpful in identifying which parameters are important in a certain problem and which observations to make to calibrate them.

**Guideline 4: Include many kinds of data as observations in the regression**

It’s also stressing the importance of using many kinds of data in the model as in guideline 2 but here specifically in the regression problem.

**Guideline 5: Use prior information carefully**

Using prior information allows direct measurement of model input values to be included in the regression or the model in general. A difference is made between model input values and observations because the latter can generally be measured more accurately. If measurements of the model input values were accurate and applicable to the scale of the model, model calibration would be unnecessary or less important. Of importance here are the aforementioned and discussed problems of scaling and heterogeneity. A parameter which is derived in the lab on 200 cm³ of sediment can not be used without serious questions for a model cell of 2000 m³. Parameters derived with field tests are better of. For instance, hydraulic conductivities derived with a pumping test represent far better an aquifer averaged value than derived in the lab. Heterogeneity is also important. Because of heterogeneity, it is not certain if a parameter derived in spot A is also valid in spot B albeit in the same layer. This was shown with a Theis-type of aquifer in chapter 6 for the case of hydraulic conductivity. Different pumping tests in
highly heterogeneous layers can lead to significant important conductivity variations. This is less the case in only moderately heterogeneous aquifers. The aforementioned scale problem of dispersivity will be always a problem. Dispersivity increases in function of travel distance towards an asymptotic value. This asymptotic value, the distance at which this value is reached and the way of dispersivity increase in function of travel distance are characteristics of the aquifer.

So, are parameter values derived with field test to be used or not in regional models despite the influence of scale and heterogeneity? The answer is certainly yes, but with precaution. The hydraulic parameters (hydraulic conductivity, specific elastic storage, storage coefficient near the water table, ...) are layer averages and can thus be used in larger models if the heterogeneity is moderately important. Otherwise, geologic knowledge of the site must be relied on. Is there trending heterogeneity, discontinuous heterogeneity, field tests on nearby sites, etc. Dispersivity values are in a different league. One must be sure that dispersivities are derived on the same scale as on which they are used in the model or at least that a asymptotic value is used. The forced gradient test discussed in chapter 5 do not results in these asymptotic values, thus they can not directly be used in a regional model. The tests do provide additional information about aquifer heterogeneity. An estimate must be made based on the derived values, knowledge about aquifer heterogeneity and testing against concentration observations.

**Guideline 6: Assign weights that reflect measurement errors**

**Guideline 7: Encourage converge by making the model more accurate**

Guideline 6 and 7 are given for the regression and are not discussed here.

**Guideline 8: Evaluate model fit**

Residuals are very helpful to evaluate model fit. Ideally, residuals are randomly distributed. Identification of trends in the residuals thus means that the model does not represent the observations well. In that case, it is often difficult to identify the cause of the problem but model error (how parameters are defined) and data errors (data entry errors or mistakes in the definition of associated simulated values) are the most frequently occurring errors.

**Guideline 9: Evaluate optimised parameter values**

Optimised parameter values must be logical and physical possible. From for instance drilling descriptions and borehole measurements, the relative ordering of conductivity values can be derived. The calibrated model must reflect this ordering. This simple test can be a powerful indicator of model error as shown by Poeter & McKenna (1995), Poeter & Hill (1997), Anderman et al. (1996) and Hill et al. (1998).

**Guideline 10: Test alternative models**

In most problems, there is more than one representation of the system possible and it is encouraged to test alternative models. Models that are more likely to be accurate tend to have a better fit, weighted residuals that are more randomly distributed and more realistic optimal parameter values.

**Guideline 11: Evaluate potential new data**

Sensitivities and correlations can be used to evaluate potential new data. If a parameter is sensitive for these data and not correlated importantly with other parameters, this parameter could be derived more accurate. If not, no effort should be made to obtain these data. Sensitivity analyses can in this context be used to identify important knowledge gaps existing to study a certain problem.
Guideline 12: Evaluate the potential for additional estimated parameters

Sensitivities and correlations can also be used to evaluate if additional parameters can be calibrated based on the available data.

Guideline 13: Use confidence and prediction intervals to indicate parameter and prediction uncertainty

Guideline 14: Formally reconsider the model calibration from the perspective of the desired predictions

These guideline is related to inverse modelling and is not discussed further here.

7.3.2 Case study: Houtave

7.3.2.1 Introduction

Many processes influence the distribution of fresh and salt water in coastal aquifers. The influence of aquifer heterogeneity and human interference such as land reclamation is illustrated in the Belgian coastal plain where, around 1200 AD, the reclamation of a tidally influenced environment was completed. The aquifer, which was filled with salt water, is thereafter freshened. The areal distribution of peat, clay, silt and sand influences the general flow and distribution of fresh and salt water along with the drainage pattern and results in the development of fresh water lenses. The water quality in and around the fresh water lenses below an inverted tidal channel ridge in the Belgian eastern coastal plain was surveyed. The hydrochemical evolution of the fresh water lens was reconstructed. The development and evolution of the fresh water lens is then modelled using a two-dimensional density depended solute transport model MOCDENS3D (Oude Essink, 2001). Results from the modelling and the chemical analyses are combined to look at the development of the fresh water lens. Finally, sensitivity of drainage levels and conductivities are studied. Thus, geological history of the area, lithology, groundwater flow, hydrochemistry and results of pumping tests are all integrated into the modelling to study the development and characteristics of a fresh water lens. With this case study, it is shown how the integration of all these data in a model leads to interesting results about the development and evolution of fresh water lenses.

7.3.2.2 Geological history

The sediments in the Belgian coastal plain have been deposited after the Ice Ages due to the interaction of sea level rise, palaeotopography, sediment supply and creation of accommodation space (Baeteman, 1985, Baeteman et al., 1999). Human activity and interaction was and still is an important component of the evolution of the coastal plain.

During the last Ice Age, seal level was between 110 to 130 m below the current level with as a result that large parts of the present North Sea laid dry. Afterwards, sea level rose due to the change in climate, for instance sea level was about 45 m below the current level 12000 years ago. At the same time, the North Sea spread towards the south again. Between 7500 and 5500 BP a mud-flat environment with mud and salt marsh deposits was formed. Tidal channels and gullies were incised in the coastal plain. Small local peat layers were formed but peat growth was severely limited by the migration of tidal channels. The groundwater reservoir was almost completely filled with salt water. Only at places were peat developed, fresh water could infiltrate to form a very shallow fresh water lens. During the Holocene, the rate of sea level rise diminished from about 3 m per 100 years between 7500 to 5500 BP to about 0.7 m per 100 years from 5500 BP on. Before 5500 PB, mainly sand and clay sediments are deposited and the mud-flat environment enlarged inland. The lower rate of sea level
rise from 5500 BP on resulted in an expansion of peat growth. The coastal peat marsh reached such a large lateral extension that by 4800 BP it dominated large parts of the coastal plain. Although most of the aquifer was still filled with salt water, a shallow fresh water lens could develop under the peat layer. Peat development continued locally to about 2000 BP. Renewed invasion of the sea ended the peat growth. Probably less sediment supply from within the North Sea was available. Former seaward deposits were eroded and are transported inland. The coastline was therefore advancing inland. The peat marshes evolved again in a mud-flat environment. Tidal channels drained the peat layer which compacted in the surroundings of these channels. Infiltration to the groundwater consisted mostly of brackish to salt water. Silting up of the coastal plain continued towards equilibrium conditions with the sea level rise and with time, channels in the mud flat did not longer expand further inland. They retreated seawards after completely silting up.

Evidence of human activity in the coastal plain is found from Roman times onward. Dikes were built, probably as early as the 10th century AD around the tidal channels. They served to protect the reclaimed land from water entering the coastal plain by these tidal channels. A dense network of drainage channels was constructed for this land reclamation, which led to further compaction of the sediments. With further habitation, most of the coastal plain became reclaimed land. Tidal channels are thought to be reclaimed from the beginning of the 12th century AD onwards (Ervynck et al., 1999). Salt water could only infiltrate the aquifer during catastrophic floodings. Under normal conditions, fresh water infiltrated the aquifer, displacing the older salt water.

Figure 7.3 Up until today, the water levels in the polders are and must be artificially regulated. Therefore, a dense network of drainage channels is present going from very small channels (A and B) draining individual pastures to larger channels in which the former flow out such as the Noordede (C) in the study area. Pumping stations then lever up water in larger channels that discharge the water in the sea. Pumping station De Steeger (D) is one of three stations in the Nieuwe Polder van Blankenberge which jack up drainage water in the channel Brugge-Oostende (photos: A. Vandenbohede).
The necessary intensive drainage and the compaction history of the sediments before and during land reclamation resulted in the still now observable geomorphology of the area. The drainage of the sandy channel deposits resulted in minor compaction of these sediments. This is in contrast to the clay and peat layers for which compaction can be considerable (for peat, to almost 50% of its thickness for the best-drained parts). Consequently, the old tidal channels formed ridges that stand above the areas where the peat layer occurs. This is best illustrated in the central part of the eastern Belgian coastal plain. This area is part of the ‘Nieuwe Polder van Blankenberg’, the second largest polder of the Belgian coastal plain. Surface level of one of the major channel ridges in this area, the Stalhille channel ridge, is between 3-4 mTAW whereas this is 2-3 mTAW for the peat areas. The geomorphology and the lateral lithological changes between peat and channel sand deposits influence the displacement of salt by fresh water. The vertical conductivity of clay and peat is much smaller than the vertical conductivity of the sandy channel deposits and because of the intense drainage, only the uppermost few metres in the areas where the peat layer occurs are freshened. The water table is approximately 0.5 metre higher on the channel ridge with respect to the surrounding areas. Thus, a fresh water lens has developed below the inverted tidal channel ridge. Beside the replacement of salt by fresh water, geochemical reactions alter the composition of the fresh water. Different chemical processes can be deduced. There are alterations of infiltration water in the unsaturated zone and mixing with seawater. Further, reactions between sediments and groundwater such as cation exchange and solution of minerals are important.

![Figure 7.4](image)

**Figure 7.4** (A) Geomorphologic map of study area (after De Moor et al., 1993) and (B) position of the 1500 ppm TDS contour line (after De Breuck & De Moor, 1975). Locations of wells and cross-sections A-A’ and B-B’ are indicated.

De Vries (1981) and Stuyfzand (1993) provide conceptual models for the Dutch coastal plain for the hydrology throughout the geological history described above. Stuyfzand (1993) also describes the hydrochemistry and its evolution for the Dutch dune area. A map showing the depth of the 1500 ppm total dissolved solids (TDS) contour line was constructed by De Breuck & De Moor (1974) for the Belgian coastal plain. This interface is found at depths ranging between less than two to maximum 30 m. The deepest positions of the interface are found under the dunes and the inverted tidal channel.
The evolution of the fresh water lens in the dunes and the particular inversion of salt and fresh water beneath a flat shore with high tidal fluctuations has been simulated by Lebbe (1999b).

**Figure 7.5** Cross-section A-A’ (a) and B-B’ (b) through the study area with lithology and position of the 1500 ppm TDS contour line.

### 7.3.2.3 Study area

The central part of the eastern coastal plain is dominated by a major tidal channel ridge, the Stalhille channel ridge. Figure 7.4A shows the geomorphologic map of the area. Figure 7.5 shows two cross-sections (A-A’ and B-B’) through the study area based on borehole descriptions and on the water quality map of De Breuck & De Moor (1974). The quaternary geological history and the geological structure of the eastern Belgian coast has been discussed intensively (De Breuck et al., 1969; Mostaert, 1985). Attention has been paid to the role of intercalated peat layers that occur abundantly in the coastal plain (Franceschi, 1975, Allemeersch, 1984) mainly as sea level indicators and paleoecological indicators. These intercalated peat layers are very important in understanding the distribution of fresh and salt water in the study area (Vandenbohede & Lebbe, 2000). The Stalhille channel ridge consists of fine sand with shell debris. Locally more silty horizons and horizons with clay pellets and/or peat fragments occur. On top, there is a clay layer with iron sulphide minerals, mainly pyrite. This clay is the upper layer throughout the area and is deposited in the period after the peat development. A 1.5 to 2 m thick peat layer is found below the clay layer and lateral to the Stalhille channel ridge. It consists of different kinds of fen and bog peat (Allemeersch, 1984). Silty to clayey fine sand with horizons of shell or sandstone debris are found below the peat layer and adjacent to the deeper part of the channel ridge. In the northern part of the study area, a clay layer is found
below the peat layer (figure 7.5). This sand, peat, silt and clay deposits make up the aquifer that is bounded below by Eocene clay and sandy clay deposits. The depths of the deposits vary because the Eocene deposits are intersected by paleovalleys. In the study area the average depth is 28 m.

Figure 7.4B shows the depth of the 1500 ppm TDS contour line in the area. This map is constructed by a network of borehole observations and geo-electrical surveys (De Breuck & De Moor, 1974). The relation between the Stalhille channel ridge and the depth of this interface is prominent. The interface below the channel ridge can be found at a depth of 20 to 25 m. The interface is shallow and positioned in the top peat and clay layers (figure 7.5A) in the adjacent area where the peat layer occurs. The area east of Stalhille channel ridge is a complex area where the peat layer has been cut up by gullies and creeks and also by historic peat cutting. Fresh water lenses formed in these channels and creeks as well. The exploitation pits of the peat cutting have been filled with a mixture of clay, silt and/or sand. These sediments with intermediate hydraulic conductivities also permit the growth of fresh water lenses. Cross-section B-B’ is situated in this area (figure 7.5B). It starts in the eastern part of the Stalhille channel ridge where the interface is deep. Adjacent to the channel ridge the interface is positioned in the top peat and clay layers as is the case in cross-section A-A’. To the west the peat layer is more cut up. Different fresh water lenses developed. Even under the peat layers the interface is pushed further in the aquifer.

7.3.2.4 Methodology

The first analyses of interface depths of fresh water lenses were carried out by Badon-Ghyben and Herzberg respectively in 1889 and 1901. They used simple hydrostatic conditions in a homogeneous coastal aquifer. Applying the Dupuit-Forchheimer approximation they independently developed a formula to predict the depth of the interface. This Badon Ghyben-Herzberg relation states that the depth of the interface is 40 times the difference of the height of the water table above mean sea level taking into account a buoyancy of 0.025. Subsequently different scholars (i.e. Hubbert, 1940; Cooper, 1959 and Glover, 1959) have shown the influence of advection and dispersion on the flow of fresh and salt water. Instead of a sharp transition zone as stated in the Badon Ghyben-Herzberg relation, dispersion results in a transition zone between fresh and salt water. The aquifer is thereby considered homogeneous in porosity and permeability. The complex structure of the coastal aquifer however makes changes of permeability and porosity very important in treating the groundwater flow. The influence of boundary conditions (drainage pattern) and hydraulic parameters (hydraulic conductivity and dispersivity) are shown here. Therefore a numerical simulation has been performed with the computer code MOCDENS3D (Oude Essink, 2001). It is based on the three-dimensional solute transport computer code MOC3D (Konikow et al., 1996), but adapted for density differences. This adaptation to a density-dependent groundwater flow model is made in the same way as Lebbe (1981) which uses fresh-water heads in a two-dimensional density-dependent model without hydrodynamical dispersion. Three-dimensional flow in MOCDENS3D is described by the following equation:

\[
\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - W = S_s \cdot \frac{\partial h_f}{\partial t}
\]

x, y and z are coordinate directions: \(q_x, q_y, q_z\) are Darcian flow velocities (m/d) in x, y and z direction; \(W\) (d\(^{-1}\)) is a flux term accounting for pumping, recharge, or other sources and sinks; \(h_f\) is the fresh water head (m); \(S_s\) is the specific elastic storage (m\(^{-1}\)) and \(t\) is time (d). The groundwater flow velocities are given by:

\[
q_x = -K_p \cdot \frac{\mu * \partial h_f}{\partial x}
\]

\[
q_y = -K_p \cdot \frac{\mu * \partial h_f}{\partial y}
\]
\[ q_z = -K_z \left( \frac{\partial h}{\partial z} + \frac{\rho_i - \rho_f}{\rho_i} \right) \]

\( \mu_f \) and \( \mu_i \) are the dynamic viscosity (kg/md) respectively of fresh water and water at the \( i^{th} \) point; \( \rho_f \) and \( \rho_i \) are the densities (kg/m³) respectively of fresh water and water at the same point; \( K_{fx}, K_{fy} \) and \( K_{fz} \) are fresh water horizontal hydraulic conductivities (m/d) and \( g \) is the acceleration due to gravity (m/d²). Fresh water heads are used to cope with the different densities of waters. Groundwater flow can be simulated in an aquifer where density differences of groundwater occur and variations in hydraulic parameters within one layer and/or between different layers can be included. The groundwater flow equation is solved by the MODFLOW code taking into account density differences using a buoyancy term \(((\rho_i - \rho_f)/\rho_f)\) in the basic flow equations. This buoyancy is related to concentrations through the equation of state:

\[ \rho = \rho_f \left( 1 + \frac{\rho_i - \rho_f}{\rho_f} \cdot \frac{C_{i,j,k}}{C_s} \right) \]

where \( C_{i,j,k} \) is the concentration (mg/l) of the \( i^{th} \) row, \( j^{th} \) column and \( k^{th} \) layer in the model, \( C_s \) is the concentration (mg/l) of salt water and \( \rho_s \) is the density of salt water (kg/m³). The advection-dispersion equation is solved by the methods of characteristics (Konikow & Bredehoeft, 1978).

Water types are determined following the Stuyfzand method (Stuyfzand, 1986) which classifies waters in main types, types, subtypes and classes using a code. The main type is determined by the Cl⁻ concentration. Fresh (F, 30-150 mg/l Cl⁻), brackish (B, 300-1000 mg/l Cl⁻), salt (S, 10000-20000 mg/l Cl⁻), hyperhaline (H, >20000 mg/l Cl⁻) and intermediate stages (Fb, Bs) are considered. Total hardness determines the type. Very soft (code 0) to extremely hard water (code 9) are considered. The most important cations and anions determine the subtype. The sum of Na⁺, K⁺ and Mg²⁺ in meq/l corrected for a contribution of seawater determines the class. With freshening the class becomes positive due to cation exchange. With salinization, the reverse is true. Using the water types, bodies of water with specific origin (hydrosomes) and prograding evolution lines along flow lines (facies sequences) can be deduced (Stuyfzand, 1999).

The chemical reactions occurring during fresh/salt water displacement can be deduced from the comparison of the calculations of conservative mixing between fresh and salt water with the water analyses. The concentration of an ion \( i \), \( m_{i,\text{mix}} \) (mmol/l), by conservative mixing of fresh and salt water is (Appelo & Postma, 1996):

\[ m_{i,\text{mix}} = f_{\text{sea}} \cdot m_{i,\text{sea}} + (1 - f_{\text{sea}}) \cdot m_{i,\text{fresh}} \]

where \( f_{\text{sea}} \) is the fraction of seawater in the mixed water and \( m_{i,\text{sea}} \) and \( m_{i,\text{fresh}} \) (mmol/l) are the concentrations of ion \( i \) in respectively sea and fresh water. Any deviation of the concentration \( m_{i,\text{sample}} \) in the sample from \( m_{i,\text{mix}} \) is due to additional chemical reactions:

\[ m_{i,\text{react}} = m_{i,\text{sample}} - m_{i,\text{mix}} \]

The fraction of seawater is calculated based on the Cl⁻ concentration of the sample (\( m_{\text{Cl}^-,\text{sample}} \)) and of fresh (\( m_{\text{Cl}^-,\text{fresh}} \)) and seawater (\( m_{\text{Cl}^-,\text{sea}} \)):

\[ f_{\text{sea}} = \frac{m_{\text{Cl}^-,\text{sample}} - m_{\text{Cl}^-,\text{fresh}}}{m_{\text{Cl}^-,\text{sea}} - m_{\text{Cl}^-,\text{fresh}}} \]
7.3.2.5 Water quality analysis

The geomorphologic map and water quality distribution map give only general information about the position of the interface. More detailed information is obtained from water extracted from observation wells. Two well nests were installed in the Stalhille channel ridge, Db14 and Db13, from which water analyses were taken for the mapping of the depth of the 1500 ppm total dissolved solids (TDS) contour line for the Belgian coastal plain (De Breuck & De Moor, 1974). Four additional wells, Sb1, Sb2, Sb5 and Sb8 were drilled. Position of these wells is indicated in figure 7.4 and screen intervals, water types, seawater factor and enrichment or depletion of \( \text{Na}^+, \text{K}^+, \text{Mg}^{2+}, \text{Ca}^{2+}, \text{HCO}_3^- \) and \( \text{SO}_4^{2-} \) with respect to conservative mixing of seawater and infiltration water are summed up in table 7.2. Db14 consists of four observation wells, Db14/1, Db14/2, Db14/3 and Db14/4. Db13 consist of two observation wells, Db13/1 and Db13/2. Four new wells were installed in and below the peat layer. Sb5 and Sb8 are situated close (± 5m) to the border of the Stalhille channel ridge: the former below the peat layer, the latter in the peat layer. Sb1 and Sb2 are situated further from the border of the channel ridge (± 200 m): the former below the peat layer, the latter in the peat layer. Water analyses are presented in figure 7.6 following a presentation method proposed by Chadha (1999). The difference in milliequivalent percentage between alkaline earths (\( \text{Ca}^{2+} \) and \( \text{Mg}^{2+} \)) and alkali metals (\( \text{Na}^- \) and \( \text{K}^- \)) is plotted on the X axis and the difference in milliequivalent percentage between weak acidic anions (bicarbonate) and strong acidic anions (chloride and sulphate) is plotted on the Y axis. As the water samples result from conservative mixing of sea water and infiltration water, composition of this mixing water for the different samples calculated based on chloride concentration are indicated on the diagram. Two main evolutions can be distinguished. A first evolution results in relatively less \( \text{Na}^- \) and \( \text{K}^- \) and/or more \( \text{Ca}^{2+} \) and \( \text{Mg}^{2+} \) and relatively less sulphate and/or more bicarbonate. A second evolution results in relatively less \( \text{Ca}^{2+} \) and \( \text{Mg}^{2+} \) and/or more \( \text{Na}^- \) and \( \text{K}^- \) and relatively less sulphate and/or more bicarbonate.

<table>
<thead>
<tr>
<th>Sample (screen interval)</th>
<th>Water type</th>
<th>( f_{\text{sea}} )</th>
<th>( \text{Na}^+ )</th>
<th>( \text{K}^+ )</th>
<th>( \text{Mg}^{2+} )</th>
<th>( \text{Ca}^{2+} )</th>
<th>( \text{HCO}_3^- )</th>
<th>( \text{SO}_4^{2-} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Db14/1 (4.8-5.8)</td>
<td>F3CaHCO3⁺</td>
<td>0.0030</td>
<td>0.310</td>
<td>0.929</td>
<td>2.717</td>
<td>-0.636</td>
<td>5.010</td>
<td>0.581</td>
</tr>
<tr>
<td>Db14/2 (12.2-13.2)</td>
<td>F3CaHCO3⁺</td>
<td>0.0047</td>
<td>0.207</td>
<td>0.834</td>
<td>2.837</td>
<td>-0.730</td>
<td>5.016</td>
<td>0.569</td>
</tr>
<tr>
<td>Db14/3 (16.1-17.1)</td>
<td>F3NaHCO3⁺</td>
<td>0.0070</td>
<td>4.045</td>
<td>1.150</td>
<td>3.272</td>
<td>-1.320</td>
<td>8.025</td>
<td>0.585</td>
</tr>
<tr>
<td>Db14/4 (23-24)</td>
<td>S4NaCl⁻</td>
<td>0.7972</td>
<td>-37.090</td>
<td>-1.309</td>
<td>8.818</td>
<td>-0.490</td>
<td>11.370</td>
<td>-6.686</td>
</tr>
<tr>
<td>Db13/1 (13.5-14.5)</td>
<td>B6NaCl⁻</td>
<td>0.1295</td>
<td>14.746</td>
<td>1.583</td>
<td>-1.178</td>
<td>-0.607</td>
<td>10.965</td>
<td>1.167</td>
</tr>
<tr>
<td>Db13/2 (21.6-22.6)</td>
<td>S6NaCl⁻</td>
<td>0.5879</td>
<td>-12.295</td>
<td>0.153</td>
<td>4.218</td>
<td>0.282</td>
<td>19.714</td>
<td>-4.094</td>
</tr>
<tr>
<td>Sb1 (8.3-9.3)</td>
<td>B3NaCl⁺</td>
<td>0.1404</td>
<td>24.299</td>
<td>1.043</td>
<td>-2.939</td>
<td>-2.564</td>
<td>21.543</td>
<td>-2.719</td>
</tr>
<tr>
<td>Sb2 (3.6-4.6)</td>
<td>B4CaClO</td>
<td>0.0438</td>
<td>-2.982</td>
<td>2.274</td>
<td>1.947</td>
<td>4.989</td>
<td>11.406</td>
<td>1.871</td>
</tr>
<tr>
<td>Sb5 (4.2-9.2)</td>
<td>F2NaHCO3⁺</td>
<td>0.0059</td>
<td>7.265</td>
<td>0.881</td>
<td>1.114</td>
<td>-2.491</td>
<td>6.021</td>
<td>-0.086</td>
</tr>
<tr>
<td>Sb8 (3.6-3.8)</td>
<td>F2NaHCO3⁺</td>
<td>0.0096</td>
<td>9.297</td>
<td>0.769</td>
<td>0.655</td>
<td>-2.718</td>
<td>6.974</td>
<td>-0.148</td>
</tr>
</tbody>
</table>

Db14/1 and Db14/2 have both a F3CaHCO3⁺ water type and a TDS (Total Dissolved Solids) of 1035 mg/l and 985 mg/l respectively. Db14/3 has a TDS of 1385 mg/l and is a F3NaHCO3⁺ water type. The deepest well contains almost pure seawater (27600 mg/l TDS) and is a S4NaCl⁻ water type. Sb5 and Sb8 have a TDS of respectively 1202 mg/l and 1402 mg/l. Both are a Fb2NaHCO3⁺ water type. Sb1 has a TDS of 6900 mg/l and is a B3NaCl⁺ water type. Sb2 is a B4CaClO water type with a TDS of 3180 mg/l. Db13/1 is a B6NaCl⁻ water type with a TDS of 6150 mg/l. Db13/2 has a TDS of 21700 mg/l and is a S6NaCl⁻ water type. Note that the transition zone between fresh and salt water observed in Db14 is small (order of metres). In Db13 this transition zone is in the order of 10 metre.

The water analyses and trends in figure 7.6 point to cation exchange as a major process determining water quality observed in well nest Db14. Clay particles are able to adsorb cations due to their negative charge. An exchange complex in equilibrium with sea water contains approximately 60% \( \text{Na}^+ \), 25% \( \text{Mg}^{2+} \), 10% \( \text{Ca}^{2+} \) and 5% \( \text{K}^- \), whereas an exchange complex in equilibrium with fresh water contains almost exclusively \( \text{Ca}^{2+} \) (Appelo, 1994). Upon displacement of the seawater with fresh
water, first the Na\(^+\) from the exchanger will be exchanged for Ca\(^{2+}\) from the water. Following Na\(^+\) exchange, K\(^+\) and Mg\(^{2+}\) will be removed from the exchanger. The expected sequence in water types along a flowline will therefore be NaHCO\(_3\), KHCO\(_3\), MgHCO\(_3\) and finally CaHCO\(_3\). In piezometer nest Db14, NaHCO\(_3\) (Db14/3) is observed in the deepest part of the lens. The CaHCO\(_3\) water type is found in the upper part of the fresh water lens (Db14/2 and Db14/1) and makes up the major part of it.

![Figure 7.6 Water analyses plotted following the method of Chadha (1999). The conservative mixing of fresh and salt water based on chloride concentration for every sample is indicated.](image)

This cation exchange scheme explains the water types and the geochemical calculations for the three uppermost screens of Db14. In the deepest part of the fresh water lens (Db14/3) a large enrichment of Na\(^+\) is encountered (4.045 mmol/l) with respect to the more shallow wells (0.310 and 0.207 mmol/l). Due to the cation exchange, a second phase of calcite solutions occurs resulting in the higher surplus of HCO\(_3\). No MgHCO\(_3\) water type is found but Mg\(^{2+}\) concentration increases downward in the aquifer as is also \(m_{\text{mg.react}}\). In all three piezometers, a surplus of SO\(_4^{2-}\) is found due to the oxidation of pyrite. Db14/4, situated under the interface, shows the reverse situation. The water is depleted in Na\(^+\) and is enriched in Mg\(^{2+}\) and HCO\(_3\). Sulphate is reduced. This water samples shows that salinization has occurred. This means that salt water has replaced fresh water. The same can be observed in Db13. Db13 is also situated in the Stalhille channel ridge but 5 km north of Db14. Seawater factor is two orders greater than for Db14/1/2/3. The mixing zone is very large in this situation. In Db13/3 there is a surplus of Na\(^+\), indicating cation exchange. Db13/2 shows, as Db14, salinization. This is due either to the interface moving upwards or this water has replaced fresh water or both. The first explication means that the fresh water lens becomes smaller. The second explication means that seawater has replaced fresh water before the reclamation of the tidal channels. The latter explication is perhaps the most likely. Before the coastal plain develop in a tidal flat environment after the Ice Ages, continental sediments were deposited and fresh water could enter the groundwater. Afterward, the coastal plain developed into a tidal flat and salt water entered the groundwater reservoir, replacing the fresh water. This points to the complex (hydro)geological history of a tidal flat area. The same applies to the larger transition zone between fresh and salt water observed in Db13. Gradually decreasing salinity of the infiltration water in comparison with the more inland situated Db14 may account for the larger transition zone.

Sb5, Sb8, Sb1 and Sb2 are presented here as an illustration of the water types found on the border of the Stalhille channel ridge and in and around the peat layer. A slightly higher TDS is found in the peat layer (Sb8) with regard to underlying sandy deposits (Sb5). As will be pointed out in the modelling
section the fresh water lens expands also laterally and the areas just adjacent to the creek ridge are also freshened. Smaller hydraulic conductivity and therefore larger residence time of the water in the peat layer results in the observed slightly higher TDS. Both Sb5 and Sb8 show a deficit in sulphate concentration (table 7.2) due to reduction reactions in and around the peat layer. Enrichment in K⁺, Mg²⁺ and especially Na⁺ indicates cation exchange as encountered in Db14/3. Sb5 has the reverse trend in the plot of figure 7.6 compared to Sb8. Sb5 has a relatively long screen (5m) in the sediments under the peat layer. It is situated in a zone where older water (type Db14/4) interacts with fresh infiltration water (see simulation). Sb1 has a TDS of 6900 mg/l and is a B3NaCl⁺ water type. It shows the same trend as Db13/2 and Db14/4. Sb2 is a B4CaClO water type with a TDS of 3180 mg/l. This later water type evolves due to salinization of the water after an initial freshening.

7.3.2.6 Numerical model of the inverted creek ridge

The lithology of the study area is very complex due to the intersection of tidal channels and gullies in the peat layer and to historic peat exploitation. Only the general outlines and positions of the peat layer, tidal channels and gullies are known. So, there are not enough lithological data to base a three-dimensional simulation of the area’s hydraulic evolution on. Additionally, the evolutions of drainage levels are not known in detail. The goal of the simulation is moreover to visualise the evolution of the fresh water lens and to study some factors influencing it. A situation as observed in the piezometer nest Db14 where the transition zone is small, is used as a reference. Therefore, with MOCDENS3D (Oude Essink, 2001) a two-dimensional steady state model is made that shows the development of the fresh water lens under the Stalhille channel ridge after land reclamation. The conceptual model for this simulation is shown in figure 7.7. It consists of 56 layers and 120 columns, so the grid has 6720 cells. Every cell has a width and a length of 5 m and the thickness of every layer is 0.5 m. So, the model grid is 600 m width and 28 m deep. It is divided into two parts (figure 7.7), the eastern side (columns 61 to 120) represents the channel ridge and the western side (columns 1 to 60) represents the adjacent clay covered area with a peat layer. The water table forms the upper boundary. The amount of infiltration is 280 mm/year. The water table is regulated by means of the drainage package in MODFLOW. Drainage levels are shown in figure 7.8. The lower boundary is formed by the Tertiary substratum, which consists of clay and sandy clay deposits. These deposits can be considered as impervious in this model and are found at a depth of 28 m. The eastern boundary is the water divide on the Stalhille channel ridge, the western boundary is a constant head boundary. The fresh water head values increase with depth. They are calculated taking into account that there is no vertical flow along this boundary. These fresh water head values correspond with the drainage level of the polder, approximately 2.0 mTAW.

Figure 7.7 Conceptual model for numerical simulation with indication of the hydraulic conductivity zones.

The first four layers are the most recent clayey deposits on top of the peat layer. The fifth to eighth layers are the peat layer in the western section and the top of the Stalhille creek ridge in the eastern section. The ninth to fifty-sixth layers are the siltsous sand below the peat layer in the western section and the creek sediments in the eastern section. Values for hydraulic conductivity are indicated on
Chapter 7: Applications of field derived parameters

A. Vandenbohede

Figure 7.7. The ratio between the horizontal and vertical hydraulic conductivity is 10. Field values for hydraulic conductivities are derived from Vandenbohede (1998) and Van Meir & Lebbe (1998). These hydraulic conductivities were derived by simultaneous interpretations of all drawdowns, observed during single or multiple pumping tests, using an inverse numerical model (Lebbe, 1999b).

At the beginning of the simulation, the groundwater reservoir is completely filled with salt water. This salt water has a TDS of 27000 mg/l and a density of 1019 kg/m³. The fresh replacement water has a TDS of 1000 mg/l and a density of 1001 kg/m³, resulting in a buoyancy of 0.018. These are the TDS values that are observed in the deepest well (Db14/4) and most part of the fresh water lens (Db14/1, Db14/2).

Land reclamation of the tidal channels must have been established during the twelfth century AD, so the simulation is run over 800 years. One stress period with timesteps of 0.5 years is considered. After each timestep, the groundwater flow is recalculated taking into account the salt-fresh water distribution from the previous timestep. Eight particles are placed per cell and the head change criterion for convergence is 0.1 mm.

Due to the sharp transition zone observed in DB14, longitudinal ($\alpha_L=0.01$m) and lateral ($\alpha_T=0.001$m) dispersivities are very small. Figure 7.8 shows the simulation results of the fresh water lens development. Figure 7.9A shows the evolution of the TDS in the middle of the channel ridge on three different depths. The fresh water lens develops relatively rapidly. In about 300 years the steady state condition is almost reached. Afterwards only minor further freshening occurs in the deepest part of the lens. Arrows in figure 7.8 are showing the velocity and direction of groundwater flow. Water infiltrates on the creek ridge and generally moves downwards. From the 280 mm/year that infiltrates, approximately 160 mm goes to the groundwater and 120 mm is drained. Deeper in the fresh water lens, groundwater flow is lateral and upwards towards the boundary of the channel ridge. Along this flowlines NaHCO₃⁺ (deepest) and CaHCO₃⁺ (shallow wells) is encountered as discussed in the hydrochemical section. Flow velocities are generally very small (in the order of $10^{-3}$ m/d). The highest velocities (in the order of $10^{-2}$ m/d) can be observed on the transition between the channel ridge and the adjacent clay and peat layers. This is the place where the water, infiltrated on the channel ridge, is drained. Groundwater flow velocities below the peat layer are very small (in the order of $10^{-4}$ m/d). Infiltration water on the clay covered peat areas is drained immediately before it can infiltrate deeper in the groundwater reservoir. This results in the upward flow below the peat layer. Freshening not only occurs under the channel ridge but also in and under the peat layer in the transition zone between the channel deposits and the peat and clay layers as indicated by the water samples. After 50 years, it can be seen on figure 7.8 that the transition zone between fresh and salt water is shifting westwards below the peat and clay layers. After 75 years, the transition zone is moving westward in both the peat and clay layers and in the layers below them. The movement of the transition zone is approximately 0.26 m/year. This compares well with the water quality encountered in Sb1/2 and Sb5/8. In Sb5/8, close to the channel ridge, fresh NaHCO₃⁺ water is found due to the replacement of salt by fresh water. In Sb1/2, placed farther from the channel ridge, brackish NaCl⁺ and CaCl₂ water is observed.
7.3.2.7 Sensitivity analyses

Three sensitivity analyses are performed to study the effect on the geometry of the fresh water lens and its formation time. The model presented in figure 7.8 and 7.9A is used as reference case. In a first
analysis, the drainage level on the clay covered peat area is set at 2.1 mTAW instead of 2 mTAW. The effect is that the head difference between this area and the channel ridge is now smaller. The depth of the interface is therefore approximately 1.75 metres less deep. Figure 7.9B shows that freshening occurs faster when the drainage level is 2.1 mTAW. The concentration contour line of 10 g/l for instance is found after 261 years in layer 33 of the model (depth is 16.25 m) whereas this is after 296 years for the reference model. The transition zones width (2 m) is the same. Lateral freshening below the peat layer occurs marginally quicker (0.272 m/y) but the extension remains the same. The transition zone width below the peat layer is, however, larger (37.5 m in comparison of 30.0 m). Less infiltration water is delivered to the groundwater reservoir, approximately 130 mm/y.

**Figure 7.9** Evolution of the TDS in function of time for layer 10 (1), 26 (2) and 33 (3), respectively 5, 13 and 16.5 m below the centre of the channel ridge. (A) is the reference model and (B), (C) and (D) are respectively the first, second and third sensitivity analysis.

For a second sensitivity analysis, the hydraulic conductivity of the Stalhille Channel ridge is 2.5 m/d instead of 5 m/d. Ratio between the horizontal and vertical hydraulic conductivity remains 10. After 800 years the depth of the fresh water lens below the channel ridge and lateral extension below the peat layer remains the same as for a hydraulic conductivity of 5 m/d. Figure 7.9C shows, however, that the time after which the fresh water lens is established is smaller. Concentration contour line of 10 g/l is found in layer 33 after 220 years. The inclination of the third curve in figure 7.9C is less than in 7.9A. The transition zone has also a width of 2 m, which confirm that the interface movement is faster. The lateral extension of the fresh water lens below the peat layer is also faster (0.312 m/y) and this lateral transition zone is smaller (27.5 m) then for the reference case. This explains why the fresh water lens is established faster. Less water is drained along the transition zone, thus more water is available for the formation of the fresh water lens than is the case in the reference model. Due to the lower hydraulic conductivity, only 110 mm/y of the infiltration water enters the groundwater reservoir.

In a last sensitivity analysis (figure 7.9D), the influence of heterogeneity in the channel ridge is studied. This is simulated by alternating layers with a horizontal hydraulic conductivity of 5 m/d with layers with a horizontal conductivity of 1 m/d in the channel ridge. The ratio between the horizontal and vertical hydraulic conductivity remains 10. As in the second sensitivity analysis, the depth below the channel ridge and lateral extension below the peat layer remains the same after 800 years but the time after which the lens is established is different. Lateral extension is faster (0.328 m/y). The concentration contour line of 10 g/l is found in layer 33 after 219 years. The same conclusions can be drawn as for the second sensitivity analysis. This shows that the time of fresh water lens formation is
determined by the least permeable layers in the aquifer in case of a heterogeneous aquifer with an alteration of permeable and less permeable layers.

7.3.2.8 Conclusions

This case study illustrates how in the Belgian coastal plain mainly aquifer heterogeneities and human interference in a complex build coastal aquifers determine the distribution of fresh and salt water. The geomorphologic map, the water quality map and the cross-sections show that the general distribution of fresh and salt water is conditioned by the presence of either peat layers, old channel ridges, creeks, gullies or historic peat exploitation pits. Below the inverted channel ridges, fresh water lenses could develop whereas salt water is still present below the peat layer.

Before the land reclamation salt to highly brackish water entered the aquifer. Influences of this water can still be found in water types under the peat layer and beneath the fresh water lens. Land reclamation of tidal channels, probably accomplished before 1200 AD, led to freshening of the aquifer. Most of the fresh water lens consists of CaHCO$_3^+$ water. Only the deepest part has NaHCO$_3^+$ water. Saline waters below the fresh water lens and the wide transition zone observed in Db13 illustrate the complex (hydro)geological history of a tidal flat and its reclamation. These saline waters show salinization. This means that either these waters have replaced fresh water before or the transition zone is moving upwards or both. The first explanation is the most probable. Before the coastal plain evolved in a tidal flat environment, depositions were continental and filled with fresh water. Afterward, in the tidal flat environment salinization occurred which explained the observed salinization still present in the water samples below the fresh water lens. The now observed fresh water lenses represents a second stage of freshening and is, in contrast to the first stage completely human induced. Besides mixing of fresh and salt water, cation exchange, calcite solution and oxidation of pyrite and organic material are the major geochemical processes determining water quality in the aquifer.

Numerical modelling shows that the establishment of the fresh water lens occurred in approximately 300 years. Sensitivity analyses show that drainage levels mainly influence the depth of the transition zone whereas the hydraulic conductivity mainly influences the timescale of the fresh water lens' formation. The exploitation of the limited fresh water supplies in the Belgian coastal planed should be studied carefully since the formation of fresh water lenses under the inverted tidal channel ridges took almost 300 years. An ill-considered exploitation of these fresh water supplies can destroy them within a very short time span.

7.3.3 Case study: The ‘Westhoek’ nature reserve

7.3.3.1 Introduction

Westhoek nature reserve

In a second case study, the groundwater flow under the dunes, shore and polder in and around the ‘Westhoek’ nature reserve is simulated. The reserve is situated on the most western point of the Belgian coast. It is a dune area of about 340 ha in size and is one of the last unfragmented dune areas along the Belgian coast. Since 1957 the Westhoek dunes are designated as a state nature reserve and are currently in hands of the Nature Department of the Ministry of the Flemish Community. It is bordered in the north-east by ‘Vissersdorp’, an allocated dune area of 60 ha and in the east by ‘Calmeynbos’, an afforested dune area of 105 ha. In the north a concrete dike between the beach and the fore-dunes forms the border. In the south, there is a low lying hinterland, a so called polder or polder area.
Figure 7.10 Location of the Westhoek state nature reserve along the French-Belgian border and the North Sea.

Geographically, the Westhoek dunes are part of the north-west European coastal dunes, which form a long, very narrow dune strip from Calais (France) to the north of Denmark. The landscape of the Westhoek dunes varies from north to south: beach – fore-dunes – northerly parabolic dune belt – mobile dune complex – southern parabolic dune belt – inner dune fringe. The beach before the Westhoek dunes is one of the widest beaches of Belgium and has a low angle dip. The coastal dunes of Belgium can be divided into ‘young’ dunes, formed between the 8th century and present and the fossil dune formed 2000 to 5000 years ago. The young dunes have lime-rich, basic or neutral soils resulting in unique flora.

The Belgian coast has a tidal dominated sandy runnel and ridge beach. The mean slope is 1.1% at De Panne. It is covered by semi-diurnal tides. The difference between the high and low tide is at spring tide approximately 5 m and at neap tide 3 m. The sea level reaches its highest point at +5.5 mTAW and its lowest point at 0 mTAW. With a frequency of about eleven cases in ten years the sea level overreaches +5.5 mTAW (Coppe & Keyser, 1967). The horizontal distance between the mean high-tide line and the mean low-tide line ranges, which is the length of the fore shore, ranges between 300 to 450 m. The length of the back shore, or the distance between the dunes and the mean high-tide line, is between 50 to 100 m. The back shore is only inundated during very high sea levels. The morphology of the shore is very dynamical and changes in time are function of sediments (grainsize, supply, etc) wave conditions (wave type, energy, wave direction, tidal range …), current shore profile and sea level. These conditions make the Belgian shore of the already mentioned sandy runnel and ridge type which is in a dynamical equilibrium.

At the end of the Atlanticum, a protective coast barrier was formed. A smaller, second dune belt (the old dunes of Adinkerke-Ghyvelde) was formed more inland before a tidal inlet which developed to a lagunal environment, the so called Moeren. This old dune belt was degraded by renewed invasion of the sea resulting in the inundation of the polder area and in the end of peat development. A new dune belt was formed more seaward from the old one (De Ceunynck, 1992). Fragments of these dunes are found in De Panne and are dated at 800 BC. Large parts of these dunes were also annihilated somewhere between 200 and 800 AD. The young dunes, the current dune belt, started to form from the 7th or 8th century on. This formation took place in several phases. The fist phase is the ‘mobile dune phase’ (9th to 10th century). Large sand drifts from the dry beach started this phase. Mobile dunes moved land inwards and a zone of 500 to 800 m wide was covered under the dune sand. When the
mobile dunes had passed, a flat to slightly undulating dune area emerged at a level of 6 to 7 m TAW, which was stabilised by vegetation. The second phase was the ‘parabolic dune phase’ in which parabolic dunes formed under the influence of the vegetation, behind the mobile dunes. The stabilising effect of the vegetation was strengthened by the groundwater level rise, which was the result of the broadening of the dune area. At the beginning of the 16th century the movement of the mobile parabolic dunes ceased. The current dune fringe is probably the result of afforestation of the dunes. The afforestation protects the polders from being covered under drift sands. In later phases the influence of people became even more important. Because of overexploitation, overgrazing, collecting firewood etc. the dunes became mobile again.

Figure 7.11. The dunes and the shore of the western Belgian coast. It is one of the few places along the Belgian coast where dunes and shore form a whole (photos: A. Vandenbohede).

The lower substratum of the phreatic aquifer is formed by clay of the Kortrijk Formation, Ieper Group. It is of early Eocene age and is considered as impermeable for this study. The lower part of the aquifer consists of medium to coarse medium sands of Eemian age. The larger part of the aquifer is formed by fine medium sands. Lenses of silty fine sands can occur. The top of the aquifer consists of medium sands. Before the urban area of De Panne a sandy layer with an accumulation of shells occurs on the back shore between the fine medium sands and the uppermost medium sands. On some places underneath the beach a silty fine sand layer is found between the lower medium to coarse medium sands and the upper fine medium sands which form a semi-permeable layer. Generally, the aquifer becomes more heterogeneous going in eastern direction from the French-Belgian border.
Past hydrogeological research

Fresh water percolates into the dune deposits and forms a fresh water lens. This fresh water body is of great importance for the dune’s ecological and biological features but it is also a major source of drinking water for the people living in the coastal zone, hence the importance of the hydrogeological aspects of the dune area.

During the period 1974-1978 a detailed hydrogeological study of the dune area west of De Panne was executed (Lebbe, 1978). Lithostratigraphy of the groundwater reservoir was studied, resistivity logs in boreholes were made, grain size analyses were performed and hydraulic parameters were deduced from pumping tests and from analyses of tidal and yearly fluctuations of hydraulic heads. Groundwater quality was studied with water sample analyses and resistivity logs. Surprisingly, salt water was found above fresh water on the shore in the area of the high-water mark. This remarkable occurrence of salt and fresh water was further studied (Lebbe, 1981). Therefore, 30 rotary drillings...
were performed on five rows or cross-sections each one perpendicular to the shore. Resistivity logs (long normal method) were performed in each of these boreholes over the 5 cross-sections. The locations of the cross-sections are given in figure 7.13 and the resistivity profiles in figure 7.14. Fluctuation of the hydraulic head in time was recorded in different shallow (P1, P2, P3, P4, P5 and P6) and deep (P2' and P4') observation wells of cross-section K0. These measurements were recalculated as fresh water heads and are given in figure 7.16. From these observation wells, water samples were extracted and analysed.

![Figure 7.14 Resistivity profiles K0 to K4 (Lebbe, 1999b).](image)

The K0 profile coincides with the French-Belgian border and a salt water lens is found above a fresh water tongue. There is a brackish transition zone with varying thickness. At the border between the dunes and the shore the transition zone is nearly vertical, the dunes being filled with fresh water. Further under the beach, the transition zone is nearly horizontal, gently rising in the direction of the sea. The thickness of the salt water lens diminishes towards the sea. The same general picture is found in cross-sections K1 and K2, being it that in K1 the fresh water evolves into brackish water towards the sea. In K2 brackish water is found underneath the fresh water towards the sea. K3 and K4 are completely different. The extension of the fresh water below the salt water is severely reduced.

All the field measurements were integrated into mathematical models. First, a 2D steady state model was made (Lebbe, 1981). Herein, a sharp interface (without dispersion) between fresh and salt water was considered and density differences were included. It showed clearly the origin of the density inversion. Fresh water infiltrates the dune area, filling these with fresh water. Due to the hydraulic gradient below the shore, fresh water flows towards the sea. There occurs thus an important submarine discharge of fresh dune water. On the back shore and the upper part of the fore shore salt water infiltrates. It forms a salt water lens that flows upon the fresh dune water. On the largest part of the fore shore the salt water flow is directed vertically upward resulting in an outflow at the beach surface. The fresh water only flows out at the sea-bottom. We have thus a deep fresh water tongue filled with fresh dune water flowing towards the sea with above it a salt water lens originating by the infiltration.
of sea water on the back shore. Diminishing of the fresh water flow from the dune area limits the extension of the fresh water tongue under the shore. This explains the K3 and K4 cross-sections. They are situated close to the urban area of De Panne where infiltration is less and where there is an important water catchment. That means that flow of fresh water from the dune area towards the sea is severely reduced.

**Figure 7.15** New, mobile equipment was developed to allow quick drilling in the dunes and on the shores. Especially on the shore, drilling is a race against the clock due to the tides. Notwithstanding the difficulties, boreholes with a depth of 30 m were made. (photo: L. Lebbe)

In a further step, a 2D solute transport model was developed (Lebbe, 1983) (figure 7.17). A mathematical model of solute transport and dispersion (Konikow & Bredehoeft, 1978) was modified so that density difference effects could be taken into account. The groundwater reservoir was treated as homogeneous. The origin and development of the water quality in function of time could be simulated. A sequence of 500 years was simulated. Initially, the groundwater reservoir is considered filled with salt water. From this point on the sea did not inundate the young dune ridge and the water starts to infiltrate driving out the salt water. After 500 years a dynamic equilibrium is reached, the quality distribution does not change any more. It reflects the situation found in K0. The observations made in K0 are thus in dynamic equilibrium. This situation is influenced more to the east by the water catchment. The influence of pumping in the dune area was incorporated. It shows the extension of the salt water lens, diminishing of the fresh water tongue and ultimately the flow of brackish and salt water towards the production wells.

In a last step a regression modelling procedure was used in which hydraulic parameters for density dependent flow and solute transport parameters were simultaneously considered with the parameters of the salinity-resistivity relationship (Lebbe, 1999b). The 2D density dependent solute transport model discussed above was used to identify relevant parameters. Resistivity measurements, fresh water head and salt water percentages were used as observations. Horizontal and vertical hydraulic conductivities were identified together with the effective porosity and the longitudinal and transverse dispersivity. The average formation factor is 3.98 and the resistivity for pure salt water and pure fresh water are respectively 0.434 Ωm and 20.1 Ωm. Matrix resistivity is 320 Ωm. It was also shown that the water collection areas are not jeopardised by sea level at the mean water line but by high water levels at the high water lines.

Recently, a 3D density dependent groundwater flow model of the shore, dunes and part of the polder was made by Luyten (2003). It is centred around the water catchment of De Panne but also includes the Westhoek nature reserve. The heterogeneity of the groundwater reservoir is included as good as is possible based on available drilling descriptions in the area. The flow under the shore is only simulated very crude because the relatively large cell dimensions (75 m * 75 m * 2.5 m). It show
Figure 7.16 Freshwater head fluctuations observed at the French-Belgian border. Location of the wells is indicated in figure 7.14 (Lebbe, 1981).

Figure 7.17 Evolution of flow, fresh water heads and groundwater quality under the dunes, shore and sea during 500 years after the formation of the dune belt (Lebbe, 1983).
among other things that the hydraulic heads in the nature reserve are minimally influenced by the water catchment. This very interesting model is not ideally suited to study flow under the shore because of the large cells dimensions.

To conclude, a system where in dynamical equilibrium conditions salt water flow is observed above fresh water is remarkable. In our knowledge, no equivalent systems have been reported in literature. However, drilling on tidal influenced beaches is not evident. It is expected that more of such flow systems exits. They can occur on other shores that have tidal influence and where a significant seaward hydraulic gradient exists under the beach (this is a relatively wide shore with a small slope). The significance of the observations and modelling is not only to shores with rather high tidal fluctuations and wave heights but can also be extended to small tidal fluctuations and wave heights as for example the Mediterranean sea (Lebbe, 1999b). The appearance of a semi-pervious layer at a limited depth will, however, reduce the infiltration of saltwater on the shore and consequently the extend of the upper saltwater lens under the shore. This is for instance the case in the unconfined aquifer at the eastern Belgian coast (Lebbe et al., 1990).

Why another set of simulations?

Past research has been very extensive, so why perform again calculations on the groundwater flow in the area? Two main reasons can be quoted, one from a ecological or nature preservational point of view, the other from a modelling point of view.

It is of no doubt that the coastal ecosystem, or the system of sea-shore-dunes-polders, is a unique one but also a very fragile one. It took until 1996 for the first management plan to be written for the Westhoek state nature reserve and it is currently being carried out. It is based on the idea of integrated coastal zone management and on the ecosystem approach. The latter states that an inventory of the past and present conditions of the coastal ecosystems (beaches, salt marshes, dunes, dune/polder transitions zones) is essential to develop ecologically sound nature management and to allow sustainable use of coastal resources. The idea of an integral coastal reserve states that within the protected area all geomorphological zonations of the coastal ecosystem are enclosed. In the protected area natural values should be maintained, restored or optimised by appropriate nature management. Other activities such as recreation and coastal defence are still allowed but will be restricted by ecological conditions.

The Westhoek state nature reserve was appointed as an intermediary landscape type, between a subdued dynamic dune landscape and a dune landscape with half-natural units. Relict or habitat management will be pursued and large areas with potentially suitable habitat will be reclaimed and extensive grazing will be used. There are also several vegetation types and fauna that are relics for Flanders, which need to be preserved, but are dependent on nature technical corrections to survive. There are two fenced areas where grazers are present for the purpose of nature management. The fences are to keep the animals away from other parts of the dunes but also to keep people out to avoid confrontations. The management plan of 1996 is currently being executed. It means that the large landscape ecological processes (major sand drift, natural evolution of the coast, spontaneous afforestation, etc) will be left to function naturally, but technical management measures (grazing, local fixation, reclamation of brushwood, etc) are necessary to diminish the negative internal and external influences like desiccation and extensive growth of brushwood.

Due to the high value and ongoing execution of a management plan, further research is certainly validated. We argue here in this context not only to look at subsystems (for instance flow under the dunes, flow under the shore, flow in the polders) but for making the link between different subsystems. The flow under the shore is for instance highly dependent on the flow under the dunes. The outflow of fresh water around the low water line may give rise to a unique fresh or brackish water minded fauna. For instance, typical fresh water nematodes (pers. comm. S. Degraer) have been found in this zone. These faunas are totally dependent on the fresh water flow from the dunes, under the
shore towards their habitat. The fresh water tongue, under the shore, seems also a promising place to look for fresh water nematodes which are washed out of the dune area. Another interesting topic is the flow in the salt water lens. Salt water infiltrates on the back shore and landward part of the fore shore and flows out at the seaward part of the fore shore. This breaks up the shore in two zones, one where the sediments going to a continuing cycle of wet and dry periods and one where the sediments are always moist or wet. These are important different conditions for organism on or in the sediments. In the former case, these organisms must be adapted to severe changes, during low tide they must survive in a moisture poor surrounding and during high tide, they must make their living in salt water.

A third example is the flora in the dunes. Studies in the dunes between Oostduinkerke and Nieuwpoort have shown that the two thirds of all plant species is related to groundwater levels (Van Der Veken et al., 1984). Water balance is thus the determining factor in the floral development of the dunes.

A second argument to do further calculations in these area is the development of more sophisticated computer codes and more powerful computers to run them on. The grid we used here is much finer than what was possible in the past. This means that the groundwater flow can be simulated in more detail. For instance the effects of tides, monthly variations in infiltration and a storm can be calculated accurately.

Evolution of the flow system and the water quality distribution are well understood. Main goal of the simulations here is to study the effects of external influences on the groundwater flow and water quality distribution. Influences which are working on different time scales are investigated. These are tides (influences of hourly sea level variations), storms (influence of extreme but short period sea levels), monthly infiltration in the dunes (variations on a monthly time scale) and sea level rise (long term sea level change). Study of these influences can hopefully lead to better understanding and appreciation of the integrated flow system under shore, dunes and polders.

First, the evolution of the salt water lens and fresh water tongue are simulated with a 2D density dependent solute transport model based on the knowledge gathered with all previous modelling exercises and compared with cross-section K0. This cross-section is least influenced by the water catchment of De Panne and reflects best the natural occurring situation. Then, sensitivity analyses of the current steady state situation are made. Main part is the simulation of the effects of tides, storms, monthly infiltration variations and sea level rise on the groundwater flow and on the water quality distribution.

### 7.3.3.2 Evolution in time of the flow system

A 2D density dependent solute transport model was made with MOCDENS3D (Oude Essink, 2001). Conceptual model of the problem, parameterisation and boundary conditions were based on the results of the above mentioned past modelling exercises. The goal of the first simulation is to make a steady state model to visualise the water quality evolution. This model can then by used as an starting point for transient flow simulations.

The model consists of 30 layers and 126 columns, so the grid has 3780 cells. Every cell has a width of 10 m and the thickness of every layer is 1.0 m (for comparison, the model of Lebbe (1983) had cells with dimensions of 30 m * 3 m). So, the model grid is 1260 m width and 30 m deep. It is divided into three parts, columns 1 to 54 represents the dune area, columns 55 to 96 the shore and columns 97 to 126 the sea. The aquifer is bounded below by clay of the Kortrijk Formation, which is considered impermeable here. The landward vertical boundary is a no-flow boundary, simulating a water-divide. The upper boundary is partially located in the dunes and partially on the shore and the sea. In the dunes a constant vertical flow boundary is assumed with an infiltration rate of 280 mm fresh water per year. A constant head boundary is set on the shore and the sea. The values of these fresh water heads were deduced from measurements on the beach (Lebbe, 1981) (figure 7.16). They range from 4.5 mTAW on the dune/shore transition to 2.36 mTAW on the shore/sea transition. Between cells 55 to 56 hydraulic head decreases with 0.12 m per 10 m seawards whereas this is 0.032 m per 10 m for cells 66
Chapter 7: Applications of field derived parameters

A. Vandenbohede

The fresh water head further seaward is the mean sea level of 2.36 m. There is recharge of salt water on the back shore and on the upper part of the fore shore. The seaward vertical boundary is a constant head boundary. The salt water head is the same over the whole depth and corresponding fresh water heads are calculated.

Like the past simulations, all layers have the same parameter values based on the experience gained with above mentioned models. Horizontal hydraulic conductivity is 10.0 m/d and vertical hydraulic conductivity is 0.1 m/d. Longitudinal, horizontal transverse and vertical transverse dispersivity are respectively 0.2 m, 0.02 m and 0.002 m. Effective porosity is 0.38. At the beginning of the simulation, the groundwater reservoir is completely filled with salt water. This salt water has a TDS of 27000 mg/l and a density of 1019 kg/m³. The fresh replacement water has a TDS of 500 mg/l and a density of 1000 kg/m³, resulting in a buoyancy of 0.019. A time period of 500 years is simulated in one stress period divided in 4000 timesteps of 0.125 year each. After each timestep, the groundwater flow is recalculated taking into account the salt-fresh water distribution from the previous timestep. Sixteen particles are placed per cell and the fresh water head change criterion for convergence is 0.1 mm.

Figure 7.18 shows the results of the simulations. After 10 years the formation of a fresh water lens under the dunes is visible. Salt water is replaced by fresh water and the beginning of the formation of the fresh water tongue under the shore is visible. An important flow exists from the dunes under the shore towards the sea. This flow drives the development of the fresh water tongue. After 80 years, salt water in the dune area is almost completely replaced by fresh infiltration water. Fresh water flows also out from the sea bed. A salt water lens exists above the fresh water tongue. Salt water infiltrates on the fore shore and flows out at the back shore. The amount of infiltration and seepage, its water quality and the pathways of infiltration water are given in figure 7.19 when a dynamical equilibrium is reached. A relatively large amount of salt water infiltrates on the back shore during high tides. This water forms the salt water lens and flows out on the fore shore. Fresh water infiltrates in the dune area, flows under the salt water lens and flows out on the sea floor. Figure 7.19 gives also an indication about the travel times of water particles. Water which infiltrates more seaward has a smaller residence time in the groundwater reservoir than water that infiltrates more landward.

Fore shore and back shore refer in the remainder of the text more generally to respectively the seaward and landward part of the shore.
Figure 7.19 The figure left gives the pathways followed by the infiltration water. Positions are given every 800 days for the red lines, every 200 days for the green lines and every 50 days for the blue lines. Figures at right give the recharge velocity (positive is infiltration, negative is seepage) and TDS of the water in the first layer of the model.

7.3.3.3 Sensitivity analyses

The general layout and geometry of the salt water lens and fresh water tongue is mainly defined by the upper boundary conditions on the shore and sea and in the dunes. The constant hydraulic heads are defined by the slope of the shore and the tidal range. The effect of these boundary conditions on the flow system will be discussed in section 7.3.3.7. But what about other parameters? Therefore, four sensitivity analyses were made. Head and concentration sensitivities were calculated according to equation 5.7. One parameter (conductivity, porosity, dispersivity or infiltration on the dunes) was changed and the calculations at the end of the last timestep were used to calculate the sensitivities. Thus the present steady state situation is studied, not the evolution of flow system in time. Although being a boundary condition, infiltration on the dunes is also included in the sensitivity analyses. The results are given in figure 7.20. First the horizontal hydraulic head was set at 12.5 m/d. In a second analysis the porosity was 0.35. Longitudinal dispersivity was 0.4 m in the third analysis and finally infiltration was set at 224 mm/y.

Fresh water head sensitivities are generally very small. Notice that porosity or dispersivity change has a small effect on the heads due to the fact that the flow is density dependent. Concentrations are generally sensitive to conductivity and infiltration. Largest sensitivities are found near the vertical boundaries of the salt water lens and the outflow area of the fresh water tongue.

The sensitivity analyses show that the parameters only influence the submarine outflow of fresh dune water. This is further worked out in figure 7.21. The amount of seepage and its TDS is given for the first layer of the model. The reference situation described in the previous section is given (basis) and compared to the different sensitivity analyses. A larger conductivity (12.5 instead of 10.0 m/d) pushes the submarine fresh outflow zone seaward. This is also the case when the infiltration is smaller (224 instead of 280 mm/y) but the outflow zone is then smaller. Porosity and longitudinal dispersivity have only a negligible small influence.
Figure 7.20 Head and concentration sensitivities for horizontal hydraulic conductivity, porosity, longitudinal dispersivity and infiltration.
7.3.3.4 Influence of tides

Mean high and low water sea levels at nearby Nieuwpoort are respectively 4.38 mTAW and 0.30 mTAW. In this section the tidal influences on the hydraulic heads are simulated. Therefore, a transient flow model is made. Initial hydraulic heads and concentrations and values for the specific elastic storages are additionally needed.

Initial hydraulic head and concentration distribution is taken from the output of the steady state model after 500 years simulation time. Specific elastic storage is taken as 0.0005 m$^{-1}$ for every layer except for the first. Specific elastic storage of the first layer is cell dependent. Under the dune area, the storage coefficient near the water table is used (0.165) and the specific elastic storage (0.0005 m$^{-1}$) under the sea. Tarhouni (1994) derived this value for the storage coefficient near the water table by the calibration of an inverse numerical model using data gathered by Lebbe (1978). During low tide, the storage coefficient near the water table should be used on the shore, whereas the specific elastic storage should be used during high tide. Hence, fore every cell located on the shore, a weighted mean value is calculated based on the duration when the particular cell is flooded and when not. These time periods are derived from field measurements (figure 7.16).

Figure 7.21 Amount of seepage and its water quality. Comparison is made between the reference situation and situations were different parameters are changed.

Figure 7.22 Sea level in function of time at Nieuwpoort (1: mean spring-tide; 2: mean tide; 3:mean neap tide).
One tidal period takes 12 hours and 26 minutes. Each cycle is subdivided in 12 stress periods. After each stress period the constant fresh water heads on shore and sea are changed according to the tidal level. Therefore, the mean tides measured on Nieuwpoort are used (figure 7.22) and are brought into the model via the general head boundary package of MODFLOW. All other properties of the model (boundary conditions, parameter values, etc) are the same as for the steady state model described in section 7.3.3.2.

Figure 7.23 shows the evolution of the flow system through one tidal sequence, starting between low and high tide. High tide occurs after 4.084 hours and low tide after 10.210 hours simulation time. Figure 7.24 shows the recharge during this sequence. This recharge is considered between model layer 1 and 2. Recharge in the dune area is very small. It corresponds with the infiltration of 280 mm/year. On the fore shore, there is infiltration or seepage depending on the tide. The same is true under the sea but the infiltration or seepage is larger than on the fore shore. Two distinct discontinuities are seen. The first is at 715 m. This is where the slope of the shore alters. The second is at about 1175 metre due to the transition from the fresh water tongue to the salt sea water.

Between the low and high tide (1.021 h on figure 7.23), there is infiltration under the distal part of the sea and seepage on the shore and landward side of the sea. Large hydraulic gradients are present under the shore. Afterwards, sea level rises and infiltration shifts towards the back shore. Just before high water (3.063 h) there is only seepage in a small zone on the back shore. The hydraulic gradients under the shore become smaller and a quite complicated gradient develops under the sea and fore shore. This is due to the interaction of the infiltration because of the increasing sea level and the upward groundwater flow from deeper in the groundwater reservoir because of the general mean steady state flow pattern. The situation at high water is depicted at 4.084 hours. There is overall infiltration now. The infiltration velocities are now largest. Afterwards, sea level falls and the zone where infiltration is found retreats seaward. Interestingly, at 6.126 hours there is seepage on the back shore, infiltration on the fore shore but already seepage under the sea. Apparently, the expected infiltration is countered by the general upward flow from deeper in the reservoir. Afterwards, there is seepage and its velocity increases towards the low tide line. The hydraulic gradient under the shore becomes larger.

Figure 7.24 shows also the recharge on three positions in function of time. At 655 m (back shore) recharge changes between 0.56 m³/d (high water) and –1.74 m³/d (just before low tide). Generally speaking, seepage is more important than infiltration except around high tide. Seepage is otherwise fairly constant. The same picture can be seen on 805 m (fore shore) but the infiltration is less limited in time. Recharge changes between 1.65 m³/d (high tide) and –2.15 m³/d (low tide). At 1105 m (under the sea) recharge changes between 2.91 m³/d (high tide) and –2.92 m³/d (low tide). Infiltration and seepage are here more evenly distributed in time. Generally from the recharge figure it can be concluded that seepage is more important than infiltration on most parts of the shore and landward part of the seabed. This underlines the steady state pattern where water infiltrates on the dunes (fresh water) and landward part of the back shore (salt water), flows towards the shore and sea. Minimal groundwater flow is seen in the steady state calculations under the sea more distally from the fresh water tongue. Therefore, infiltration and seepage are more or less in equilibrium.

Evolution of drawdown in function of time is calculated for 12 observation wells (Figure 7.25). Observation wells 1, 2 and 3 are situated in the dune area. During one tidal sequence hydraulic heads in these wells do not change importantly. Wells 4, 7 and 10 are located in the first layer, representing a filter placed just beneath the surface. Wells 4,5 and 6 are placed under the back shore. Only during high tide, the water level is higher than the topographical level of the shore, therefore hydraulic head does not change considerably in well 4. Wells 5 and 6 show larger changes with time. There is also an important lag between the time of high tide and the time on which highest heads are calculated in the observation wells. This time lag (see table 7.3) is 2.042 h for well 4 and is diminishing deeper in the groundwater reservoir. This time lag is due to the large storage coefficient near the water table and the hydraulic resistance between the general head and the node of the cells of the first layer. Wells 7, 8 and 9 are situated under the fore shore. Here, time lag increases deeper in the groundwater reservoir. The evolution of the heads shows a distinct asymmetrical pattern. Heads rise quickly with rising sea
Figure 7.23 The evolution of the flow system through one tidal sequence, starting between low and high tide.

level and are largest short after high tide. Afterwards, there is an asymmetric fall in hydraulic head. The same can be seen in observation wells 10, 11 and 12 situated under the sea. This asymmetric fall is due to the mean upward groundwater flow (as calculated with the steady state model) countering the decrease of the sea level boundary condition. Notice that the time lag is larger on the back shore than below the sea because in the storage in the first layer is larger (heavily weighted towards the storage coefficient near the water table) in the former situation.

Figure 7.26 shows the movement of particles placed in the groundwater reservoir at locations indicated in figure 7.25 (points 4-12). Generally speaking, in all situations the movement is dictated by the steady state flow. The effects of the tides are superimposed on this. Starting point for the calculations is between low and high tide. Tidal effects are minimal in point 4, 5 and 6. For the other points, high tide is characterised by a downward movement of the water particles, resulting in a dip or even a loop in the particles track. The vertical deviation from the particles track is, however, small.

During one tidal cycle, groundwater flow changes considerably. This is calculated here for the first time for the shore bordering the Westhoek nature reserve. The distribution of fresh and salt water, however, is not affected by the tides. Therefore, the changes are too small and occur too quickly. The
hydraulic heads fluctuate around long term mean hydraulic heads. It is the long term steady state groundwater flow which defines the water quality distribution.

Figure 7.24 The recharge through one tidal sequence, starting between low and high tide.

<table>
<thead>
<tr>
<th>time lag (hour)</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.042</td>
</tr>
<tr>
<td>5</td>
<td>1.532</td>
</tr>
<tr>
<td>6</td>
<td>1.532</td>
</tr>
<tr>
<td>7</td>
<td>0.511</td>
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<tr>
<td>8</td>
<td>1.021</td>
</tr>
<tr>
<td>9</td>
<td>1.021</td>
</tr>
<tr>
<td>10</td>
<td>0.000</td>
</tr>
<tr>
<td>11</td>
<td>0.000</td>
</tr>
<tr>
<td>12</td>
<td>0.511</td>
</tr>
</tbody>
</table>

Table 7.3 Time lag as observed in the different observation wells.
Chapter 7: Applications of field derived parameters

7.3.3.5 Effects of storms

North-east and south-west are the most frequent occurring wind directions on the Belgian coast. The strongest winds most frequently are west-south-west winds. The most severe storms in the Belgian coastal area are thus also western storms. These storms results in temporarily large sea water levels.
The effects of these storms on the groundwater flow in the dunes and under the shore are simulated in this section.

Figure 7.27 gives some statistical information on the occurrence of larger than mean sea water levels. Therefore, gauge measurements of the period between 1925 and 1980 are used. They were kindly delivered by the ‘Ministerie van de Vlaamse Leefgemeenschap, departement Leefmilieu en Infrastructuur, administratie Waterwegen en Zeewezen’. Figure 7.27A shows for every year the highest recorded sea level. Figure 7.27B gives the distribution of these sea levels. It can be seen that the most occurring high sea water level is around 5.5 mTAW. Thus a normal mean western storm increases the sea level to around 5 mTAW. Only exceptionally, there are a few years where no such storms occur and the highest recorded water level is around 5 mTAW. Some years have seen more severe storms where the water level rose to 6 mTAW or even more. In that, the historically well know storm of 1953 is exceptional. Water levels rose above 6.5 mTAW. Figure 7.27C shows the mean largest sea level recorded between 1925 and 1980 for every month and figure 7.27D gives the frequency with which highest annual water level are recorded in a certain month. The highest water levels are found during the autumn, winter and spring and most storms obviously occur also in this period. Storms happening during the summer period are less severe.

Table 7.4 shows the frequency in which extreme water levels occur (Probabilitas n.v., 1999).

<table>
<thead>
<tr>
<th>Frequency</th>
<th>Mean Sea Level (mTAW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 per year</td>
<td>5.46 mTAW</td>
</tr>
<tr>
<td>1 per 10 years</td>
<td>5.95 mTAW</td>
</tr>
<tr>
<td>1 per 50 years</td>
<td>6.28 mTAW</td>
</tr>
<tr>
<td>1 per 100 years</td>
<td>6.41 mTAW</td>
</tr>
<tr>
<td>1 per 1000 years</td>
<td>6.86 mTAW</td>
</tr>
<tr>
<td>1 per 10000 years</td>
<td>7.28 mTAW</td>
</tr>
</tbody>
</table>

Figure 7.27 Statistical information of the occurrence of larger than mean sea water levels.

With global change in mind, it is interesting to look at the evolution of storm frequencies and associated water levels in time. Figure 7.28A shows sea levels during all recorded storms between 1928 and 1990. Figure 7.28B shows for every decennium during this period the number of storms and the mean sea level of them. In 44 out of the 48 cases, water levels stay below 6.0 mTAW. The storm of 1953 has the highest recorded water level. Interestingly, the highest storm water levels averaged over periods of 10 years do not change significantly. The mean in the period 1928 to 1990 is 5.66
mTAW. Perhaps there is an increase in the number of storms. For instance 14 storms are recorded during the seventies, whereas this is 5 during the thirties. However, during the eighties, again only 6 storms are recorded. But in 1990 alone, 6 storms were observed. So, from the available measurement no clear increase over a long period in the occurrence of storms and the associated high water levels can be deduced. Significant increases on shorter time scales seem to be very import. The mean water level during storms over a long period is more or less constant, but individual storms can deviate considerably from this level. The same is concluded by Bijl (1996) who investigated storm conditions for north-western Europe.

Perhaps interesting to note is that as a critical high tide, the levels 5.70 mTAW, 5.55 mTAW and 5.45 mTAW are considered respectively in Nieuwpoort, Oostende and Zeebrugge.

![Figure 7.28](image)

**Figure 7.28.** Water levels during all recorded storms between 1928 and 1990 (A) and for each decennium during the period 1928-1990 the number of storms and the mean sea level of them (B).

Due to its exceptionality, the effects of the 1953 storm are simulated here. The model lay-out is the same as in the previous section (7.3.3.4). The ‘Ministerie van de Vlaamse Leefgemeenschap, departement Leefmilieu en Infrastructuur, administratie Waterwegen en Zeeuwen’ kindly provided us tidal gauge measurements made in Oostende during the event. These are used as boundary conditions with the general head boundary package and are given in figure 7.29. The simulation starts at January 27, 3h00 (time 0 in all following figures). In the next days, water levels are higher then the mean tidal fluctuations (figures 7.22 and 7.25), for instance the low water levels are larger than the mean 0.3 m. From January 30 19h00 (time 101 in figures), water levels rose to result in the dramatically high value of 6.95 mTAW on February 1 2h00 (119 h).

Figure 7.29 gives also the hydraulic heads as would be measured in observation wells 4 to 12, located as in the previous section. Wells 1-3 under the dunes don’t show considerable change and are not included. The evolution of the hydraulic heads in the first 100 hours is the result of tidal fluctuations and the same conclusions as in the previous section can be made. During the storm, water levels in well 4 becomes larger than in wells 5 and 6 meaning that due to the exceptional large sea level important recharge is taking place here. The zone were recharge is taking place is pushed more towards the dune area. This is quite obvious when figure 7.30 is compared with figure 7.24. On the shore, in the mean tidal range situation 56.18 m³/d infiltrates normally during high tides. This is now increased with 61.4 % to 90.68 m³/d. The difference is largest on the back shore and diminishes toward the fore shore. The infiltration on the shore and under the sea is, however, diminished from 138.54 m³/d in the mean tidal range situation to 122.26 m³/d due to the smaller infiltration under the sea bed. Note also the important seepage of salt water in the most seaward part of the dune area during high water due to the abnormal high water level. Seepage on the shore during low tide is considerably larger than normal, 100.75 m³/d versus 47.3 m³/d in the case of the mean tidal range situation. The largest differences are found around 715 m, where the gradient of the shore changes. Seepage differences under the seabed are very small.
Figure 7.29 Sea water levels just before and during the storm of 1953 and the hydraulic response on 12 fictive wells. The location of the wells is the same as indicated in figure 7.25.

Figure 7.31 shows the movement of particles placed in the groundwater reservoir at points 4 to 12. The first part of these tracks is the same as in the mean tidal range situation and the same conclusions can thus be made. The movement of the water particles becomes somewhat more ‘chaotic’ during the storm. In wells 4, 5 and 6 particles move towards the dunes due to the high sea water level, forcing a more landward flow under the back shore. Afterwards, the particles resume their general movement. Particles 7, 8 and 9 move more upward during the storm. This is due to the increased seepage under the shore. Particle 10, 11 and 12 move in loops during the storm and afterwards upward and seaward.

A storm alters the hydraulic heads and thus also the groundwater flow. A storm cause larger than normal hydraulic heads in the groundwater reservoir. During a short time period a large amount of salt infiltrates. This salt water, however, is picked up by the general steady state flow pattern and its effects on the general water quality distribution is minimal. Calculations here are performed with one important supposition: the coastal defence prevents the sea from invading the dunes during the storm. When the sea invades the dunes, salt water will infiltrate in the dunes’ fresh water lens.
Chapter 7: Applications of field derived parameters

Figure 7.30 Recharge and general flow pattern during largest high and subsequent low tide of the 1953 storm.

Figure 7.31 Movement of particles in the groundwater reservoir.
7.3.3.6 Influence of monthly infiltration variations

Rainfall in the coastal area is typical between 750 to 800 mm/year. Obviously, there are monthly variations. The effects of these variations are calculated here. Monthly rainfall varies between 35 and 90 mm. Typically, February is the driest month whereas October is the wettest month. From meteorological data, the amount of infiltration from the total rainfall can be calculated. Lebbe (1978) provides such infiltration data from January 1957 to March 1976. These are calculations based on observations from the nearby weather station of the Koksijde Air Force Base following the method of Penman (1948). During the winter, most of the rainwater infiltrates causing the rise of the water table. In most cases, heads are largest at the end of the winter. Evapotranspiration is large during the summer and no or a very limited amount of water reaches the water table. At the end of the summer heads are mostly the lowest. In the low-lying parts of the dune area, infiltration water reaches the groundwater relatively quickly and the response of the water levels is almost instantly. This is not the case for the higher parts of the dune area. Infiltration towards the groundwater takes some time and a reaction of the water levels can be delayed by one or two months. This is, however, systematically the case for high groundwater levels not for low levels. Data from July 1970 to March 1976 are used here (figure 7.23). In figure 7.23 January 1970 is taken as time 0, just to compare different figures.

**Figure 7.22**: A: yearly infiltration in the dune area in function of time. B: Distribution of monthly infiltration during the period 1957-1976.

Figure 7.22A shows the annual infiltration (mm/year) of rainwater towards the groundwater reservoir. Data between 1957 and 1976 are from Lebbe (1978) and data between 1985 and 1994 are from Ampe & Langohr (1997). These values vary between 503.3 mm/year in 1960 and 115.6 in 1971. The mean value is 260 mm/year with a standard deviation of 110 mm/year. Figure 7.22B shows for every month between January 1957 and March 1976 the infiltration. Infiltration is largest from late autumn to early spring and is very small during spring and summer. Large differences can be found in different years.

Here, the infiltration rate in the dune area is changed following an annual pattern and the changes in hydraulic head and concentrations are simulated. Therefore, a transient flow model is made. Initial hydraulic heads and concentrations and values for the specific elastic storages are additionally needed. Initial hydraulic head and concentration distribution is taken from the output of the steady state model after 500 years simulation time and the specific elastic storages are the same as used in sections 7.3.3.4 and 7.3.3.5. A period of 81 months (6 years 9 months or 6.75 years) is simulated. So, 81 stress periods are used each divided in 2 time steps. The amount of infiltration is altered during each stress period. The rest of the parameters and the boundary conditions are the same as in the previous sections.

The simulation starts in the middle of a dry period that is close to a situation where the heads reach their average values. Figure 7.23 shows the results of the calculations. Groundwater flow is shown in
February and September of the third modelled year, this is respectively in the middle of a recharge period and in the middle of a dry period. During the recharge period an important downward flow exits in the dunes. This flow is far less pronounced during a dry period and no important head gradients exits in the dune area. The lay-out of the fresh water tongue and salt water lens is in general not affected by monthly variations in infiltration. Head and concentration variations are further studied in twelve fictive observation wells indicated on the grid (1 to 12). The largest annual head fluctuations are found in wells 1, 2 and 3 located in the dunes. Heads are large during recharge periods, small during dry periods and the succession of dry and wet periods is nicely reflected in the head fluctuations. Difference between largest and smallest levels is around 30 cm. There is a retardation between high infiltration rates and high water levels. For instance, infiltration is large at 1.0 year and the subsequent large hydraulic head is observed at 1.13 year. This is due to the large value for the storage coefficient near the water table. This retardation will be smaller in case of a smaller storage coefficient near the water table. October of year four was an unusual wet month with an infiltration of 201.4 mm. This is clearly seen in the hydraulic heads, which are importantly larger. The hydraulic heads in the dune area stay larger than normal until the next dry period. Thus a period with larger than usual rainfall and infiltration can have important consequences (i.e. larger water levels) for a relatively large period. Observation wells 4, 5 and 6 show also annual variations but of smaller amplitude (12 cm for well 6 for instance). Very small fluctuations can be seen in wells 8 and 9 but the wells are located too far seaward to record significant variations. The other observation wells do not show important fluctuations.

Variations of TDS in function of time for the different wells are also calculated. Obviously, observation wells located in of the dunes (wells 1, 2, 3), fresh water tongue (wells 6, 9, 10, 11) or salt water lens (well 7) do not show major variations because the general distribution of fresh and salt water does not change. Only observation wells located in or near transition zones show variations indicating small movements of these zones. Observation well 12 shows the most important fluctuations. This well is situated in the transition zone between the fresh water tongue and seawater. The position of this transition zone thus shifts cyclically in response with the varying infiltration. Small variations can also be seen in well 8 and minor variations in well 5, both located on or close to the transition zone between the fresh water tongue and salt water lens. Unlike the head changes, the relation between concentration changes and infiltration is not so obvious. The most radical change in quality is seen in well 4, 9 months after the infiltration peak of October of year 4. TDS drops temporarily from 27000 mg/l to 18430 mg/l. This well is located close to the transition zone between fresh dune water and the salt water lens. Due to strong infiltration the transition zone moves seaward making the well more brackish.

Conclusions of these simulations are that infiltration variations can be observed in the dunes’ hydraulic head but diminish quickly seaward. A period with large rainfall and subsequent large infiltration can result in larger than normal hydraulic heads until the next summer. The general distribution of fresh and salt water is not altered importantly. Only small variations around transition zones occur.
Figure 7.23 Results of the transient flow model simulating annual infiltration variations.

7.3.3.7 Future sea level change and change in coastal morphology

Climate Change and Sea Level Rise

During the 20th century, atmospheric concentrations of carbon dioxide and other greenhouse gases have risen substantially. These concentrations will continue to increase if no urgent and concerted action is taken to reduce emissions radically. Increase of atmospheric greenhouse gas concentrations will result in extra warming of the Earth’s surface. At this point, certainty and unanimity of opinion cease. There is much uncertainty on the assessment of the likely scale, pace and geographical distribution of the warming and other climatic changes. It is not the intention of this section to overview earth’s climate, climate change and the discussion concerning it. Interested readers are referred to Warr & Smith (1995) providing an easily accessible introduction to this complex subject.

The IPCC (Intergovernmental Panel on Climate Change) has put together four alternative visions of the future (Houghton et al., 1990) based on two important determinants of greenhouse gas emissions: the projected growth of the world population and economic growth rates for different countries or regions. One of these scenarios is the ‘Business as Usual’ (BaU) scenario. It tries to answer the question ‘What if few or no active steps are taken to limit the release of CO2 and other greenhouse gases and other conditions (little is done to promote energy-saving measures, world energy supplies remain heavily dependent on fossil fuels, tropical deforestation continued, …) remain the same?’.

Other scenarios assume rapid improvements in energy efficiency. On basis of the BaU, greenhouse forcing could reach values equivalent to a CO2-doubling by around 2020, and go on increasing thereafter. As a result, the next century could see global warming at a rate with current estimates in the
range 0.2 to 0.45 °C per century. This would be unprecedented since the planet emerged from the last glacial period some 10000 years ago. Obviously, many questions and uncertainties remain by different future climate predictions and its effects. For instance, earth’s feedback mechanisms are or may well be poorly understood and demographic, economic, social, technological and maybe above all political forces are changes hard to predict. But the message is quite self-evident: the more urgent and concerted control policies, the slower and less marked global warming is likely to be. That is the essence of the precautionary principle.

Fluctuation of sea level is one of the consequences of atmospheric temperature change. Two sorts of effects are considered: thermal expansion of seawater and the melting of land-ice. If oceans warm, the density of the seawater decreases and the oceans expand (a thermal expansion), giving a rise in sea level. There are two basic problems in predicting how much the sea level will rise: the lack of sufficient data on ocean temperature, salinity and density at various depths on a global scale and the limitations of predictions how these values vary with changes in global mean surface temperature. Land-ice volume does not necessarily decrease with rising temperature. Whether an ice-sheet gets larger or smaller, as the temperature rises, depends on the balance of two factors, the accumulation of snow onto the ice-sheet and the ablation of ice from it. At low-temperatures, below about –8°C, accumulation is greater than ablation and the ice-sheet increases in size. At higher temperatures, ablation is greater than accumulation and the size of the ice-sheet decreases.

Results of these effects are not everywhere the same. Local change of sea level depends on mentioned global factors but also regional and even very local factors determine the sea level changes at a certain place.

Based on future temperature rises, sea level rise is predicted. Table 7.5 gives estimates based on IPCC BaU policy scenario, in which few or no active steps are taken to limit the release of greenhouse gases. On that basis, the best estimate is that the sea level would be 18 cm higher in 2030 than in 1985, but could be as little as 9 cm or as much as 29 cm higher. This means a sea level rise of about 40 cm per century. Thermal expansion of water is the major contribution to with the melting of glaciers and small ice-caps as a close second. Indeed, most valley glaciers (such as for instance in the Alps) and small ice-caps (such as for instance in Scandinavia and Iceland) have decreased in size over the last 100 years. The response time of these ice masses on changing global temperatures is quite small, in the order of about 50 years or so. Contribution to sea level rise of Greenland and Antarctic ice-sheets is small because of the longer response times. The amount of ice in the Antarctic ice-sheet is enormous, about ten times as much as the Greenland ice-sheet and sufficient to cause a rise in sea level of around 65 m, if it all melted. However, this is very unlikely to happen on a short time-scale because of the long response time. It is thought that the ice-sheet hasn’t even adjusted to the last glacial-interglacial transition that ended 10 000 years ago. The climatic situation of the Antarctic ice-sheet differs also from most other ice-sheets: it is much colder. This has a considerable effect on the response of the ice-sheet to global warming, leading to the possibility that global warming could increase the size of the Antarctic ice-sheet, contributing to a fall in sea level. Hence the negative sign in table 7.5.

<table>
<thead>
<tr>
<th></th>
<th>low</th>
<th>best estimate</th>
<th>high</th>
</tr>
</thead>
<tbody>
<tr>
<td>thermal expansion of oceans</td>
<td>6.8</td>
<td>10.1</td>
<td>14.9</td>
</tr>
<tr>
<td>glaciers/small ice-caps</td>
<td>2.3</td>
<td>7.0</td>
<td>10.3</td>
</tr>
<tr>
<td>Greenland ice-sheet</td>
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<td>1.8</td>
<td>3.7</td>
</tr>
<tr>
<td>Antarctic ice-sheets</td>
<td>-0.8</td>
<td>-0.6</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>8.8</td>
<td>18.3</td>
<td>28.9</td>
</tr>
</tbody>
</table>

By 2070, the best estimate is a sea level rise of 44 cm (with a range of 21-71 cm) and by 2100 the best estimate is 66 cm (with a range of 31-110 cm). The rise is thus slightly accelerating. In the next hundred years from now the sea level rises four times faster than the last hundred years. It is this possibility of a rapid rate of global mean sea level rise, as well as the size of the rise, that is causing
Sea level rise may not rise uniformly around the world: it is likely to be influenced by local and regional land movements, which may be large and could exacerbate climate-related global changes.

Sea level rise of the North Sea

The predicted sea level rise is, in the framework of earth’s geological history very small. During the Cretaceous for instance, sea level was about 300 metres higher than now and during the last glacial, it was about 130 metre lower. So why bother? Rise of sea level predicted over the next century is, however, a very real and present danger, capable of destroying cities, croplands, coastal environments and even nations. About 50% of the world’s population lives in coastal areas, a figure which will probably rise to 75% during the first century of the second millennium (Finkl, 1994). Sea level rise and global change in general may alter hydrology of those regions considerably. Good management of the water balance and the precious fresh water resources to anticipate on the changes is therefore crucial.

As mentioned before, local sea level rise can differ considerably from the global prediction of the IPCC. Crustal movements and redistribution of surface loads are important contributions. They do not alter the amount of water in the oceans but the position of land relative to the sea level is affected. The result on land is a transgression or regression. It is know that sea level of the North Sea has, generally speaking, constantly risen after the last ice age. This rise was decelerating. Before 7500-7000 years BP, sea level rose with about 7 m/ka (Denys & Baeteman, 1995). From 7500-7000 BP to 5500 to 5000 BP this was about 3.0 m/ka. Afterwards sea level has risen with 0.7 m/ka. Two major periods of deceleration of the rise were thus found, between 7500-7000 BP and between 5500-5000 BP. Lambeck & Johnston (1995) made a glacio-hydro-isostatic model calculating the ongoing responses of the Earth to the last deglaciation and to the concomitant addition of water into the world’s oceans. The adjustment of land is not restricted to the regions close to the former areas of glaciation. Immediately beyond these regions the crust is subsiding, primarily in response to the glacial unloading of the crust in former glaciated areas. Further away the dominant adjustment of the crust is to the water load added into the oceans during the melting of the ice-sheets. The large sea level change just after the last ice age is due to melting of large volumes of ice and due to glacio-hydro-isostatic processes. Afterwards, the latter is the dominant factor. These authors calculated that the current sea level rise due to glacio-hydro-isostatic adjustments is about 5 cm per century for the Belgian coast. From measurements it is know that between 1900 and 2000, sea level has risen 15 to 20 cm in Belgium. No acceleration of this rise is observed (Van Cauwenbergh, 1999). Jelgersma (1992) found that sea level has risen during the past centuries before 1900 with a rate of 5 to 6 cm per century and the Dutch RLG (1998) (Raad voor het Landelijk Gebied) found a rate of 3 to 5 cm per century. These values compare well with the rise calculated by Lambeck & Johnston (1995). So, the rise during the last century is about 4 times larger than before. According to Jelgersma (1995) this higher rate is due to a global temperature rise. According to the RLG (1998) this acceleration is an effect caused by the Little Ice Age (1450-1850). What about the future? In Belgium, a sea level rise of 60 cm per century is taken into account in the construction of new coastal infrastructure.

Different scenarios are considered in calculating the effect of sea level rise on the groundwater flow under the polders, dunes, shore and sea of De Panne. In a first scenario, a coastal defence (for instance dike) is present so that the sea does not gain on the land. The morphology and level of the shore stays the same but the seaward extension of the shore is diminishing in time. Its morphology and level is altered in a second scenario. In a third scenario shore and sea retreat landwards whereby the dune belt becomes narrower. The rate of sea level rise for all calculations is 0.4 m per century. This is in line with the BaU policy of the IPCC. However, no acceleration is considered.

A change of sea level rise has consequences not only on the seaward facing dunes, shore and sea but on the whole dune area and also in the polder area. Therefore, the model used until here is enlarged,
incorporating the total dune area and part of the adjacent polders. This enlarged model (polder-dune-shore-sea model) is presented and discussed first in the next section. It is a steady state model.

Presentation and discussion of polder-dune-shore-sea model

The polder-dune-shore-sea model is the same steady state model as described in section 7.3.3.2 but extended towards the polder area. So four domains are modelled, the polder area, dune area, shore area and sea area respectively with a width of 750, 1700, 540 and 300 metre. The model has 30 layers and 330 columns, resulting in a grid of 9900 cells. Each cell has a width and a length of 10 m and the thickness of each layer is 1.0 m. So, the model grid is 3300 m width and 30 m deep. A constant fresh water head boundary is present in the first layer (3.0 mTAW for the first 500 years and 2.4 mTAW afterwards) in the polders and in the first column. The fresh water head values of the first column increase with depth. They are calculated taking into account that there is no vertical salt water flow along this boundary.

Parameter values under the dunes, shore and sea are the same as in the previous models. The horizontal hydraulic conductivity of the polders is 6.5 m/d for layers 3 to 30 (Van Meir & Lebbe, 1998). The top of the polder groundwater reservoir is made up of a less conductive layer. The horizontal hydraulic conductivity for the layers 1 and 2 is 3.25 m/d. Anisotropy or the ratio between horizontal and vertical conductivity remains 100. A time period of 700 years is simulated in two stress periods, each divided in timesteps of 0.125 year. After each timestep, the ground water flow is recalculated taking into account the salt-fresh water distribution from the previous timestep. The first timestep is 500 years long, the second 200 years. This is done to incorporate the drainage history of the polders. The simulation starts after the reclamation of the polder, certainly accomplished at 1300 AD. Before 1800, the drainage level was higher than the current one. This level is estimated to be around 3.0 mTAW. Afterwards, drainage levels were lowered due to the construction of the canal Veurne-Duinkerke and the Langeleed to around 2.4 mTAW. The Langeleed is situated along the dune-polder boundary and was specially constructed to drain the water flowing from the dunes towards the polder area.

Before going to the results of the modelling an important issue, the position of the dunes’ water divide, is illustrated with a simple analytical model. The hydraulic head in the dunes (h_x in m) in function of the distance x (m) to the high water line is given by (Van Der Veken et al., 1984):

\[ h_x = -\frac{N}{kD} x^2 + \left( \frac{h_2 - h_1}{B} + \frac{NB}{kD} \right) x + h_1 \]

where N is the infiltration (m/d), kD is the transmissivity (m²/d), B is the width of the dunes (m), h_1 is the high water level of the sea (m) and h_2 is the water level in the polders (m).

For all calculations B is 1710 m, kD is 300 m²/d (or 10 m/d times 30 m) and N is 280 mm/year. Three situations are calculated. In the first scenario (scen1) high water level of the sea is 4.5 m and drainage level in the polders is 3.0 m. In the second case (scen 2) the drainage level is altered to 2.4 m. Due to the smaller drainage level in the polders the water divide shifts 70 m seawards, from x = 680 m in scenario 1 to x = 610 m in scenario 2. This means that more water flows from the dunes towards the polder area and less towards the sea. The lowering of the drainage levels in the polders thus logically have a drawback: more water must be drained. In a third scenario (scen 3) due to sea level rise, the high water level is increased to 6.5 mTAW. The water divide is found at 390, or shifted 220 m seaward. A relatively large amount of water thus flows less towards the sea but instead towards the polders.
Chapter 7: Applications of field derived parameters

Figure 7.34 Results of the calculation of hydraulic head in the dunes with an analytical model. The high water line is at \( x=0 \) and the dunes are 1710 m in width. Three different scenarios outlined in the text are calculated.

This analytical model is of course very simple, it does not take into account the interaction with flow under the shore and polders. Further, it is assumed that flow is predominantly horizontal, which is not the case along the boundaries of the dunes. It only provides some general information on how the hydraulic heads and water divide respond to changes in sea level and/or water level in the polders. A change in the position of the water divide means that more or less water flows towards the sea and the polders. This will have its effects on the flow under the shore and sea and on the position of the transition zone between fresh and salt water under the dune-polder boundary. This is further deduced by the numerical model.

Figure 7.35 shows the evolution of groundwater flow and quality under the polders, dunes, shore and sea. Starting point of the model is 1300 BC. As was the case in section 7.3.3.2, the groundwater reservoir is completely filled with salt water. It is further assumed that besides the lateral development of the fresh water lens under the dunes, the groundwater reservoir under the polder area remains filled with salt water, or otherwise stated that all fresh rainwater is drained away immediately. As discussed in section 7.3.2 this is a simplified view. The top of the groundwater reservoir in the polders can be filled with fresh water and due to sedimentological and morphological reasons, a complex distribution of fresh and salt water can develop. This is, however, beyond the goal of these calculations here. Moreover no major gullies, creeks or channel ridges which could result in a fresh water lens occur in the model domain as was the case in the Houtave case study.

Fresh water infiltrates in the dune and polder area but is drained immediately in the latter. Salt water infiltrates on the shore and under the sea. Drainage level in the polders is 3.0 mTAW. Evolution of the fresh water tongue and salt water lens under the shore is obviously very similar as in figure 7.18. Comparison after 500 years with this latter figure shows that the salt water lens is here less extended vertically. This is due to the position of the water divide in the dunes 720 m from the shore. In the previous calculations this distance was 500 m meaning that in the model here more water is flowing towards the sea resulting in a smaller salt water tongue. When the polder drainage level is lowered to 2.4 mTAW (from 500 years onward) the water divide shifts to 620 m from the shore, the salt water lens enlarges because fresh water flowing from the dunes towards the sea diminishes.

A relatively sharp transition zone develops between the fresh dune water and salt polder water. This transition zone shift laterally in the polders with time, creating a seepage zone of fresh water in the dune-polder border.
Figure 7.35 Past evolution of groundwater flow and water quality from 1300 BC onward.
Figure 7.36 shows the evolution of recharge and TDS along the first layer of the model. Two parts of this profile are highlighted, the polder-dune border and the shore. The evolution of the transition zone is best seen on the distance-TDS curve. Two conclusions can be made. First the width of this transition zone enlarges in the polders in time although it remains relatively sharp. This width is about 30 m after 10 years, about 50 m after 40 years and about 90 m after 160 years. Afterwards, this width does not enlarge much. Secondly, the average velocity with which the fresh water lens invades the polder is diminishing in time. This is about 2 m/year between 10 to 20 years and 0.05 m/year between 500 and 700 years. The position of the transition zone, about 250 m from the polder-dune border, is in good agreement with observations by Lebbe et al. (1983). The recharge-distance curve shows in more detail the evolution of the seepage along the polder-dune border. The largest seepage is located directly adjacent to the dune area diminishing rapidly laterally away from the dunes. The seepage at a certain point increases slightly after the transition zone has past there. For instance after 40 years, transition zone is around 700 m (distinctive bend in the distance-TDS curve) and the seepage is larger than before. The same can be said about the other curves. So, upward flow increases slightly once in the seepage zone of the fresh water lens. Interestingly, seepage does not alter very much by changing the drainage level in the polder. There is only a very small increase around 500m due to the lateral movement of the transition zone. Lowering of the drainage level thus has as effect that more water flows towards the polders (due to the shift in the position of the water divide in the dunes) but it is spread over a larger area so that seepage velocities remain more or less constant. Of course, more water must be drained in total. The seepage in the polders after 500 years is 6461 m³ per year. This rises slightly to 7298 m³ per year after 700 years. These figures are for a polder surface area of 750 m times 10 m or 7500 m². Most of this seepage water is fresh water, flowing out adjacent to the dune area.

The recharge-discharge on and around the shore is also considered in detail. On the back shore there is infiltration of salt water. This is the origin of the salt water lens under the shore. The extent of this infiltration zone is rather limited and the mean infiltration velocities are very large. On the larger part of the shore there is seepage of salt water. The change of the shore gradient is again clearly seen by a zone were the seepage of salt water is largest. More seaward fresh water flows out originating from the dunes flowing through the fresh water tongue. The distance-TDS curve of figure 7.36 shows the widening and the small seaward shift of this fresh water seepage zone. It starts as a small salt to highly brackish zone after 10 years. After 160 years it has almost reached its present day state. After 500 years it enlarges only slightly laterally: the shore facing sides its position is about the same but the sea facing side has shifted seaward. Lowering of the polder drainage level has as effect that the fresh water seepage zone shifts seawards. This is due to the smaller amount of water infiltrated in the dunes which flows towards the sea. The salt water lens is able to become larger and pushes the fresh water outflow.
zone more seawards. The distance-recharge curves can be divided in two stages. Recharge stays approximately the same during the first 20 years. Then first brackish and afterwards fresh water flows out and seepage increases. The curve of 40 years is a transitional situation.

Figure 7.36 Evolution of recharge and TDS along the first layer of the model.

Sea level rise scenario 1: dike is present and the level of the shore remains unaltered

In this first scenario it is assumed that a coastal defence is present, most likely a dike. Other, more ‘natural’ defences such as stabilisation of the coast can also be considered here. Whatever the coastal defence is, the dunes are protected for encroachment of the sea, mean sea level will rise against this defence and the width of the shore will diminish in time. No heightening of the shore is considered. This is modelled by changing the constant head boundary of the first layer on the shore and sea. The situation after 100, 250 and 500 years of sea level rise of 0.4 m per century is calculated as a steady state situation. Figure 7.37 shows the results. The current situation (700 years) is given as a reference.

Two processes occur because of the sea level rise. First, there is a shift seaward of the water divide in the dunes meaning that less fresh water flows towards the sea. The water divide is displaced seaward because the sea level becomes higher changing the dunes boundary conditions. Normally, this has as effect, as pointed out in the previous section, the enlargement of the salt water lens. The fresh water
Figure 7.37 Effects of sea level rise according to scenario 1 after 100 (800 years), 250 (950 years) and 500 (1200 years) years from the current situation (700 years).

tongue is pushed deeper in the groundwater reservoir and its seepage zone shifts more seaward. The movement of the water divide is, however, small. A piece of shore is still present between the dune boundary and the rising sea level on which the hydraulic heads do not change. A different situation arises after 500 years of sea level rise. The shore is now totally absent, boundary conditions of the dunes are directly changed and the water divide moves considerably seaward. What does influence the extent of the salt water lens here is the decrease of the width of the shore. This has as result that the water cycle forming the salt water lens (infiltration on the back shore and seepage on the fore shore) is much shorter, decreasing the extent of the salt water lens. After 500 years of sea level rise the salt water lens is completely disappeared. The tides result now only in a vertical movement of the sea
against the coastal defence. The horizontal movement of the sea between high and low tide line are absence and thus is also the salt water cycle on the shore. All what is left is a fresh water seepage zone under the sea directly adjacent to the dunes. This is the classical textbook picture of a fresh water lens under the dunes with adjacent seepage zone, here in the polders and under the sea.

The effect of a shifting water divide is also visible on the transition zone between fresh dune water and salt polder water. After 100 and 250 years of sea level rise, this transition zone stays in the same place. A small effect of the small amount of water flowing to the polder is the steeping of the transition zone deeper in the groundwater reservoir. After 500 years the transition zone has moved about 20 m landwards.

**Sea level rise scenario 2: dike is present and the level of the shore is altered**

In the second scenario it is assumed again that a coastal defence, most likely a dike, is present. Now the shore is heightened with the same amount as the sea level rise. Such a situation can be the result of regular sand suppletion on the shore and near off-shore. For instance after 100 year, the sea level will have risen by 0.4 m and the constant heads on the shore will be raised by the same amount. This is modelled by changing the constant head boundary of the first layer on the shore and sea. The situation after 100 and 250 years of sea level rise of 0.4 m per century is calculated as a steady state situation. Figure 7.38 shows the results. The current situation (700 years) is given as a reference.

Although comparative to scenario 1, a totally different picture arises. Because the shore heightens in parallel with the sea level, the boundary conditions of the dunes are changed directly. The movement of the water divide is larger than in scenario 1 resulting in a smaller flow of fresh water from the dunes towards the sea. Additionally, an important hydraulic gradient between the back shore and the sea is preserved by the fact that the level of the shore follows the sea level rise. This enables the salt water lens to become larger. Notice also that the seepage zone of the fresh water tongue becomes smaller in function of continuing sea level rise due to the smaller amount of fresh water flowing from the dunes towards the sea.

The flow of fresh water towards the polders increases. The transition zone moves about 30 m deeper in the polder and the deepest part of the zone becomes steeper.
Figure 7.38 Effects of sea level rise according to scenario 2 after 100 (800 years) and 250 (950 years) years from the current situation (700 years).

Sea level rise scenario 3: a retreating coastline

In this scenario the coastline reacts on the rising sea level with a retreatment: the width of the shore remains constant but it moves inland. The transition between polder and dunes does not change meaning that the width of the dune belt decreases. For simplicity the movement of the shore inland is equal to the transgression of the sea. When for instance the sea gains 50 m on land, the shore moves 50 m inland and the dunes are reduced with the same amount. Additionally the shore is heightened in parallel with sea level rise. When sea level rises with 0.4 m then the shore will also be heightened by 0.4 m. These are obviously simplifications. The coastal morphology is a complex interaction between tidal influences, wind climate, currents, sea level rise, topography, sediment supply, creation of accommodation space, human interference, etc.

The constant head boundary of the first layer on the shore and sea is used to model scenario 3. The situation after 100, 250, 375 and 500 years of sea level rise of 0.4 m per century is calculated as a
steady state situation. Figure 7.39 shows the results. The current situation (700 years) is given as a reference.

**Figure 7.39** Effects of sea level rise according to scenario 3 after 100 (800 years), 250 (950 years), 375 (1075 years) and 500 (1200 years) years from the current situation (700 years).
The most important factor determining the flow and distribution of fresh and salt water is the position of the water divide in the dune belt. After 100 years of sea level rise (800 years in figure 7.39) sea level and level of the shore are 0.4 m higher. This means that the water divide moves in the direction of the sea. Less fresh dune water flows towards the sea, the fresh water tongue becomes less thick and the salt water lens becomes thicker. Note also that the fresh water tongue’s seepage zone is pushed seaward relative to the new high-water line than is the case in the present situation (700 years). So, due to the sea level rise the salt water tongue becomes larger, laterally as well as vertically. At a certain point in time, the salt water lens will reach the bottom of the groundwater reservoir eliminating the outflow from fresh dune water to the sea. This can be seen after 250 years (950 years). The water divide has shifted to the border between the dunes and the shore. The fresh water tongue disappears. A deep groundwater flow cycle of salt infiltration water on the shore is present instead of the salt water lens and fresh water tongue. Almost all fresh water infiltrating on the dunes flows towards the polder. A transition zone develops between the fresh dune water and the salt infiltration water on the shore. This transition zone makes that a little amount of fresh water still flows to the sea, highly mixed with the salt water to brackish water. This brackish water flows out under the sea. A 125 years later (1075 years) there is only salt water under the shore, infiltrating on the back shore and flowing out on the fore shore and under the sea. The fresh water lens under the dunes is smaller because the infiltration zone decreases. There is already brackish water under the fresh water lens. Notice also the asymmetrical nature of this fresh water lens. It is deeper towards the polders. This is due to the dunes’ boundary conditions: the constant head on the shore is larger than the constant head in the polder. The reduction of the fresh water lens has also as a result that a small amount of salt water, which infiltrates on the back shore, flows under the fresh water lens towards the polders. The same trends are visible after another 125 years (1200 years in figure 7.39). The extent of the dunes’ fresh water lens is further decreased and the brackish outflow zone under the sea has disappeared. Note that the hydraulic head gradient under the dunes increases with time due to the higher sea level.

Figure 7.40 Evolution of recharge and TDS along the first layer of the model for scenario 3.
Figure 7.40 shows the recharge and TDS of the first layer along the profile. Only the two most important zones (polder-dune transition and the shore and sea) are presented. The recharge-distance curves on the shore show very well its retreat. Note that the infiltration velocity on the back shore increases because of the rising sea level. Notice how the seepage zone of the fresh water tongue develops. At 800 years, the current pattern of a wide seepage zone with at the shore side a gradually declining seepage and at the seaside an abrupt ending seepage is present, only shifted inland. At 950 years the seepage zone has shrunk to a very small zone but it is now brackish water which flows out. Further seawards the seepage velocity now gradually declines. There is thus a small difference between the seepage pattern when the salt water lens and fresh water tongue is present and when there is only a salt water flow cycle under the shore and sea.

TDS-distance curve for the transition between polder and dunes shows the movement of the interface between fresh and salt water. Until 950 years the transition zone moves towards the polders, 40 m in 250 years time. Afterwards the transition zone moves towards the dunes because of the shrinking fresh water lens under the latter. It moves about 210 m in the next 250 years. Total seepage in the polder area (10* 750 m²) increases importantly with time. It is 655600, 687700, 772800, 904000 and 931400 m³ per year respectively at 700, 800, 950, 1075 and 1200 years. At 700, 800 and 950 years this is almost completely fresh dune water. At 1075 and 1200 years, an important part (41 % and 63 % respectively) is salt water. When the fresh water lens under the dunes shrinks then the salt sea water will flow out in the polder area which will stress these areas considerably.

Influences of coastal morphology

The above presented calculations are interesting in the framework they are performed, namely sea level rise. However, they are even more interesting if every calculation is looked at individually because they show the behaviour of the flow systems with different boundary conditions. In this way it learns us a lot about the dynamics of the fresh water – salt water distribution in the polder-dune-shore-sea area.

The contributing factors to this distribution are:

- **The location of the water divide in the dune belt.** This determines the amount of water infiltrating in the dune area that flows to the sea and to the polders. A shift of this water divide has its consequences in the polder area and on the shore. When the water divide shift towards the sea, more water flows towards the polders. The transition zone between fresh dune water and salt polder water moves further in the polder widening the fresh seepage zone adjacent to the dune belt. Concurrently, less fresh water flows towards the sea. More salt water can infiltrate during high tide and the extension of the salt water lens (laterally as well as vertically) enlarges. The thickness of the fresh water tongue and the width of its seepage zone decreases. The position of this water divide is dependent of the dunes’ boundary conditions, the heads in the polder and on the shore. When they are the same than the water divide is halfway in the dune belt. When the head in the polder is lower than on the shore than the water divide is closer towards the sea. This is illustrated clearly in figure 7.38 where the width of the shore does not change but its hydraulic head does in accordance with sea level rise. Figure 7.40 (1075 and 1200 years) shows a situation where the width of the dune belt is limited in extend and the height difference between hydraulic head in the polder and on the shore is large. This results in a water divide on the border between dunes and shore. Almost all infiltrated fresh water flows from the dunes towards the polder. Even salt water infiltrated on the shore flows under the dunes’ fresh water lens towards the polders. No salt water lens and fresh water tongue is in this situation present under the shore.

- **The tidal range and topographic shore gradient.** These are expressed by the horizontal distance between the high- and low-tide line and the hydraulic gradient between them. The topography of
the shores along the Belgian coast is smooth and the tidal amplitude is large. This gives rise to the flow cycle in the salt water lens: infiltration on the back shore and outflow on the fore shore and in the near offshore zone. If the distance between high- and low-tide line becomes smaller, as is the case in figure 7.38 then this flow cycle becomes less important and the salt water lens becomes smaller. Ultimately on a coast where there is no shore (for instances coasts with a cliff) or the tidal range is very small (for instance inland sea) no salt water lens will be present. This is the typical textbook picture from the interaction between fresh and salt water. Only a seepage zone adjacent to the water line is present.

One thing which was not investigated in previous calculations is the effect of the topography of the shore. Change of the gradient can not be done without changing the width of the shore. Here, the width of the shore is decreased to 330 m (instead of 540 m). The slope for the first 100 m is unaltered 0.0112 and is 0.005 (instead of 0.0032) for the rest of the shore. All other model parameters and boundary conditions are the same. The results are presented in figure 7.41.

![Figure 7.41](image)

**Figure 7.41** Effect of a change in the topographic gradient on the beach. The upper figure is the current situation.

The water divide in the dunes does not change in position because the dunes’ boundary conditions do not change. The polder drainage level and the high-tide level are the same. The salt water lens becomes deeper but decreases in lateral extend. This is because the fact that about the same amount of salt water infiltrates (14.5 m³/d) on the back shore in comparison with the current situation.

### 7.3.3.8 Conclusions

A fresh water tongue is found under a salt water lens on the shore in the Belgian western coastal plain. This unique distribution is in a dynamic equilibrium. Some new aspects of this flow system were here studied. The goal of the simulations in this dissertation was to look at the groundwater flow under the
sea, shore, dunes and polder area. Especially the influences on water quality distribution and hydraulic head variations were of interest. Influences on different time scale are studied. These are tides, storms, monthly infiltration variation and sea level rise. Tides, storms and monthly infiltration variation lead to transient head fluctuations and variations in groundwater flow. These variations are fluctuations around a long term mean situation. Therefore, the distribution of fresh and salt water is not altered importantly.

Tides are sea level variations on a very small time scale. This results in a cycle of infiltration of salt water during high tide and seepage of it during low tide. This is also visible in the groundwater flow and hydraulic head pattern below the shore and sea. These fluctuations do not result in variations in water quality distribution. The time scale is therefore too short.

A heavy western storm was simulated using tide gauge measurements of the 1953 storm. It shows the influence of it on the hydraulic heads and on the groundwater flow. An important extra amount of salt water infiltrates on the shore. Part of this flows landwards. Due to its relatively short duration even a major storm as the one of 1953 has no major effect on the distribution of fresh and salt water.

Monthly variations of infiltration influence the hydraulic heads and groundwater flow. Large infiltration during the winter can lead to large heads in the dunes until the next summer. Influence on the water quality distribution is, however, minimal. Small variations can only be observed in the transition zones. As was the case for tides and storms, monthly variations causes fluctuations of hydraulic heads around a long term steady state situation. It is this long term situation which defines the water quality distribution.

Future sea level scenarios are simulated. These calculations show clearly that the flow pattern and the distribution of fresh and salt water is mainly determined by the boundary conditions, these are the drainage level in the polders, sea level, tidal range and morphology of the shore. The former two conditions determine the position of the water divide in the dunes. With the infiltration the position of the water divide defines the amount of water which flows towards the sea and towards the polders. The fresh water flow from the dunes to the sea determines the amount of water which infiltrates on the higher parts of the shore and determines at the same time the geometry of the fresh water tongue and salt water lens under the shore. The width of the shore on which salt water can infiltrate is function of the tidal range and the slope of the shore. This influences also the geometry of the salt water lens and consequently the fresh water tongue. Altering one of the boundary conditions can have important consequences for the water quality distribution and flow pattern in general. This was illustrated with the different sea level scenarios but the value of the simulations goes beyond just these scenarios.

The Westhoek nature reserve and the sea-shore-dunes-polder system in general are important from an ecological point of view. Changing the boundary conditions has its implications on the groundwater flow and water quality but subsequently also on the unique flora and fauna. Additionally, the dunes are a very important fresh water reservoir. It is the only source of fresh water in the coastal area. As a consequence these fresh water resources must be safeguarded for future generations. The calculations here have shown that major human interference can cause severe damage to the natural occurring flow system. So, these interferences should be carefully considered beforehand.
8.1 Introduction

Solute transport is of concern in many practical problems faced by hydrogeologists. Examples are the distribution of contaminants in groundwater, remediation issues, salt water intrusion issues, protection zones around production wells, etc. Besides qualitative descriptions of the stated problem quantitative answers are often required.

Hereby, modelling is an important step in the search for good and practical solutions. The complexities and interactions of processes in groundwater reservoirs are thereby included in the model as good as is possible. A modelling exercise must therefore be seen as a synthesis of all available current relevant knowledge and data on the stated problem. This includes field data (general geological data, stratigraphy, sedimentology, geological history, hydraulic and solute transport parameters, borehole measurements, water analyses, etc) but also current knowledge of the relevant processes (advection, dispersion, diffusion, chemical reactions, microbiology, etc). The fact that modelling shows relations between processes, parameters and observations is an important surplus value it can provide in a research. The fact that the complexities of a groundwater reservoir can be translated in numbers and these can be used to run simulations with, is a strong indication that, at least, the fundamental characteristics of a problem are understood.

Models need, however, a lot of input such as a good schematisation of the groundwater reservoir, based on geological knowledge; boundary conditions; hydraulic, solute transport and geochemical parameters; etc. The observations to calibrate the model are not so abundantly available. This creates two difficulties with which the practical modeller is confronted:

- Reliable parameter values are needed, first of all hydraulic conductivities of all layers, but also values for the specific elastic storages, storage coefficients near the water table, dispersivity, porosity, retardation, reaction rate coefficient, etc. In most cases these are not readily available and must thus be estimated. Therefore, it is important that field tests are designed that are easy to perform and with which reliable parameter values can be inferred. This is the subject of the first part of this dissertation. We argue here for the use of field tests. A combination of a pumping test and a tracer test was used in this research to derive hydraulic and solute transport parameters. This was first discussed from a theoretical point of view and then illustrated with three field tests. Further a test aiming to study which chemical reactions occur in the groundwater reservoir and to derive first-order reaction rate coefficients, is discussed. This test was illustrated with one practical example.

- Parameter values which are derived with a certain test or which are found in the literature can not be used in for instance groundwater flow models without any considerations on their applicability. An important characteristic of groundwater reservoirs, this is heterogeneity, should be taken into account. Typically, layering can be distinguished in many groundwater reservoirs. Each layer has its own sedimentological characteristics. These can also vary within a single layer. This has as result that a hydraulic conductivity measured at location X can be different on location Y albeit it is derived in the same layer. One consequence of aquifer heterogeneity is that parameters may
vary according to the location where they are derived. A larger degree of heterogeneity means a larger variance. It is impossible to determine the exact spatial distribution of parameter values. This should be taken into account in the model. A second consequence of heterogeneity are scaling issues. Parameter values are dependent on the scale of their inference. This is very well documented by theory and field observations for dispersivity and in lesser extend for hydraulic conductivity. Dispersivity increases in function of the scale.

Second part of this dissertation deals with applications of parameter identification tests. The applications are divided in two categories based on its scale. The application can be on the same scale as the parameter identification test, indicated as a field scale. This is for instance the case in many remediation studies. Relevant parameters are derived on the same scale as the remediation technique. In regional groundwater flow models the volume of aquifer for which a parameter is applied is larger than the scale on which it is derived.

An application in the context of the design of a remediation technique and two regional flow models are discussed. These last two aim to illustrate the characteristics of the groundwater flow and solute transport in the coastal aquifer of Belgium.

8.2 Parameter identification tests

8.2.1 Forced gradient tracer test

Different tests are available to derive hydraulic and solute transport parameters. For instance, permeameter tests, consolidation tests, well tests, pumping tests and calibration of regional groundwater flow models are all well know methods to derive hydraulic parameters. Different kinds of tracer tests are available to infer solute transport parameters. An important remark must be made concerning the scale on which the parameters are derived. Permeameter tests, consolidation tests and tracer tests performed in the laboratory use only small volumes of aquifer material. Applicability of the results is therefore quite limited. Well tests are field tests but the volume of tested aquifer material is also small and the results are highly influenced by the construction of the well. Calibration of groundwater flow models has its own intrinsic problems using it as a parameter identification tool. The derived parameters are in many cases quite unreliable and are depending on model characteristics.

Therefore we argue here to develop and perform reliable field tests. These have many advantages. First of all, groundwater flow and solute transport are studied on the scale they occur in nature. Further, parameters are derived on relatively large volumes of aquifer material. The scale of the test is also not too large so that the boundary conditions are well known and can be more or less controlled. Two interesting tests are considered: pumping tests and tracer tests.

During a pumping test, water is extracted from a permeable layer and the drawdowns are measured in this and in the surrounding layers. Horizontal and vertical conductivities, specific elastic storages and the storage coefficient near the water table can be deduced. These are average layer values. With the software package used here, HYPARIDEN (Lebbe, 1999a), layered heterogeneity can be included in the interpretation. These tests do not give detailed information about the layered heterogeneity on a small scale (decimetre scale) and about lateral heterogeneity.

During a tracer test performed on a field scale, a tracer is injected in the groundwater reservoir and its evolution in time is followed. This leads to the inference of dispersivity values. Travel times of the tracer are also deduced. These depend on the ratio of hydraulic conductivity to effective porosity. Effective porosity must be known or must be estimated to derive hydraulic conductivity or vice versa.

With a forced gradient tracer test, it is aimed to combine the advantages of pumping and tracer tests and to eliminate their disadvantages. The test consists of two steps. First water marked with a tracer is injected in the groundwater reservoir. Water is then extracted from a nearby well and the tracer plume moves from the injection well towards the pumping well. The distance between these two wells is in
the order of 5 to 10 metres. Observation wells are present between the pumping and injection well to monitor the movement of the tracer plume. Drawdowns as well as concentration measurements are made. With these two data sets hydraulic and solute transport parameters can be derived based on one field test.

The observations of drawdowns and concentrations can be performed together. Alternatively this two data sets can be collected in two steps. First a pumping test is performed and drawdowns are recorded. Thereafter the forced gradient tracer test is done and concentrations are measured. For practical reasons this last option was chosen for the field tests discussed in this work.

8.2.2 Collection of the observations

Drawdowns are measured by means of pressure transducers in the observation wells. Concentration observations are obtained by means of geophysical borehole measurements. This is related to the tracer that is used. Main objective of the tests is to study advective and dispersive transport. Therefore a non-reactive (or conservative) tracer is used, namely salt water. This was injected in groundwater reservoirs filled with fresh or brackish water. An important difference in electrical conductivity between the salt injection water and the natural occurring groundwater thus existed. EM39 measures the electrical conductivity of the sediments around non-conductive observation wells by means of a focussed electromagnetic induction method. This has as benefit that measurements can be done in already encased boreholes. The vertical resolution of the EM39 is large. Measurements with a depth interval of 20 centimetres are made resulting in a detailed vertical log of the tracer passage around the observation well. This is an important advantage with regard to other observation methods as for instance by means of water analyses.

EM39 conductivities can be recalculated in total dissolved solid concentrations of the pore water in a straightforward way. This is not the case, however, when the matrix conductivity becomes too important.

8.2.3 Interpretation of the forced gradient tracer test

Drawdowns are interpreted using the software package HYPARIDEN (Lebbe, 1999a) with which single and multiple pumping tests can be simulated and interpreted. It is constructed around a 2D axi-symmetric numerical model. The groundwater reservoir is subdivided in a number of layers. Every layer is characterised by a value for the horizontal and vertical hydraulic conductivity and for the specific elastic storage. Layered heterogeneity can thus be included. Every layer is lateral homogeneous and subdivided in a number of coaxial rings centred around the pumping well. Drawdowns are calculated in the nodal points of every ring. Inner and outer radiuses of the rings form a logarithmic series. Drawdowns are thus also calculated very accurate close to the pumping well. The groundwater reservoir is bounded on top by the water table and by an impermeable layer at the bottom.

Main advantages of numerical models such as HYPARIDEN are its flexibility and the accuracy of the calculations. This is not found in well-know and much used analytical models. These models make use of simplified groundwater reservoir schematisation with a limited number of permeable and semi-permeable layers. The groundwater flow is then less accurately calculated. For instance, hydraulic leakage or the flow of water from semi-permeable layers towards the pumped layer may severely be underestimated. Result is that the hydraulic conductivity of the pumped layer is overestimated.

Concentration observations are interpreted with the aid of TRACER3D, specially made for this study. It simulates the density dependent groundwater flow and solute transport in the vicinity of a pumping and injection well. It uses results of calculations with HYPARIDEN as a basis. With HYPARIDEN drawdowns are calculated in function of place in the reservoir and in function of time. With these
drawdowns seepage velocities are calculated and these are used to simulate solute transport by means of particle tracking. Further the method of characteristics MOC (Konikow & Bredehoeft, 1978) is applied to simulate advection and dispersion. Finally, the model calculates concentrations as would be observed with the EM39.

Interpretation of drawdowns and concentrations is an iterative process. First the drawdowns are interpreted with the inverse model in HYPARIDEN and hydraulic parameters are deduced. Then these results are used to simulate the concentration observations and solute transport parameters are deduced. This is one iteration. When necessary a number of such steps are made.

8.2.4 Applications: Houtave, Zevergem and Tessenderlo test sites

A first forced gradient tracer test was performed at the Houtave test site, situated in the eastern coastal plain. This test aimed to investigate the concept of the test, to obtain a data set to apply TRACER3D and to illustrate the advantages of the test. The test was done in quaternary sediments that have mainly a layered heterogeneity with a less important lateral heterogeneity.

A second test was done at the Zevergem test site, situated south of Gent. The groundwater reservoir consists of quaternary deposits of the Scheldt river and these are relatively heterogeneous. Aim of the test was to perform a forced gradient test in relatively heterogeneous sediments. Therefore two injection wells were used and the behaviour of both plumes was followed.

A third test was performed at the Tessenderlo test site in Limburg. The groundwater reservoir consists of glauconite rich sands of tertiary age. In contrast with the two other tests which had pure scientific reasoning this test was done in the framework of a remediation study. The site is contaminated with 1,2-dichloroethane (1,2-DCA) and a clean-up strategy had to be developed. Therefore, the contaminated part of the reservoir was characterised for its flow and solute transport properties.

8.2.5 Results of the forced gradient tracer tests

The feasibility of a forced gradient tracer test was shown at the Houtave test site. It was also illustrated that TRACER3D is capable of simulating the test’s observations. It is thus a useful interpretation tool. Horizontal and vertical conductivities of the pumped and surrounding layers, the specific elastic storages of the pumped and surrounding layers, the effective porosity and longitudinal dispersivity were deduced.

With the EM39, measurements were made with a depth interval of 20 centimetres. This means that tracer breakthrough curves are available with a depth interval of 20 centimetres in every observation well. Analysis of these curves allowed getting a qualitative idea of the heterogeneity of the groundwater reservoir. This was done for all field sites.

Comparisons of pumping and tracer test results are hard to find in literature. The agreement between these results is often problematic. The hydraulic conductivity derived with a pumping test is in many cases larger than when derived with a tracer test. This has important implications on the calculations of travel times of solutes in groundwater reservoirs. The pumping tests are, however, in most cases almost always interpreted with an inadequate analytical model. Hydraulic leakage for instance may severely be underestimated in this way. Consequence is that the hydraulic conductivity of the pumped layer is estimated too large. The three tests discussed in this work show that pumping and tracer test data can lead to corresponding results, whenever the pumping test is interpreted with an adequate model simulating the flow towards the pumping well accurately. This was illustrated in depth with the Houtave test site data. The pumping test was interpreted with some analytical models resulting in conductivity values which were too large. Consequence is that tracer breakthrough was calculated too early using these parameter values.
This does not mean that differences between pumping and tracer test results can not exist in for instance groundwater reservoirs with important 3D heterogeneities or reservoirs with a dual porosity. Especially the lack of knowledge about the exact geometry of these heterogeneities and the question how to implement them in a model are causes of possible non-agreements. This is less the case in mainly layered heterogeneous deposits as were investigated in this study.

The advantages of a forced gradient tracer test were illustrated with sensitivity analyses. These showed that hydraulic and solute transport parameters are derived more accurately when both concentration and drawdown observations are used. It was also shown that transverse dispersivity can not be derived with the test even if an observation well placed laterally from the line injection well – pumping well is used. It can even be questioned if transverse dispersivity can be derived at all with such kind of tests. The fact that very few values are found in literature confirms this.

The Zevergem test site confirmed the general conclusions from the Houtave test site but now for a more heterogeneous groundwater reservoir. Influence of heterogeneity was clearly pointed out by the fact that the two tracer plumes behaved completely different. This was due to variations in hydraulic conductivity and longitudinal dispersivity. The advantages of the combined interpretation of drawdown and concentration data were clearly illustrated. It was not possible to derive the hydraulic conductivity of a permeable layer from the pumping test. These layers are preferential pathways for solute transport and its characterisation is thus important. This value was derived with the combination of both data sets.

The Tessenderlo test site consists of glauconite rich sands. This means that matrix conductivity must be included in the conversion of EM39 conductivities to total dissolved solid content of the pore water. The matrix conductivity was estimated using EM39 measurements made before the injection of the tracer. It was presumed that the formation factor and the pore water conductivity were constant for all sediments.

An interesting result of the modelling is the fact that less injection water and tracer must be used in the simulation than was actually the case during the test. The difference is a massive 56%. Tracer breakthrough curves, however, show tailing. An important amount of tracer stays behind in a tail which moves very slowly towards the pumping well. Tailing can not be simulated in TRACER3D and a smaller amount of tracer was thus needed in the simulations. Different explanations for this tailing can be quoted. For instance hydraulic properties of glauconite are not well understood. Flow of salt water through glauconite rich sediments may alter the hydraulic conductivity. Future research on the hydraulic properties of glauconite must certainly be encouraged. Otherwise the relation between EM39 conductivity and total dissolved solids was calculated perhaps oversimplified. Relations between matrix conductivity, sediment conductivity and pore water conductivity in general and for glauconite rich sediments in particular are even so an interesting field for future research.

Geophysical borehole measurements were not only used to obtain detailed concentration observations but also to study the groundwater reservoir. Logs of natural gamma and electrical conductivity were used together with drilling descriptions in the schematisation of the groundwater reservoirs. They provide information about the clay content of sediments and thus indirectly about the hydraulic conductivity. By performing borehole measurements in different wells, an idea about the heterogeneity of the site can be obtained. This was fully incorporated in the interpretation of the forced gradient tracer tests.

8.2.6 Longitudinal dispersivity

Dispersivity is a very difficult parameter to derive and to use because of its scale dependency. This was illustrated by Gelhar et al. (1992). These authors provide an overview of publicised dispersivity values before 1992. Dispersivity increases with scale (or perhaps better with travel distance of the solute) towards a more or less constant asymptotic value. Sediment properties define this evolution. One of the conclusions of Gelhar et al. (1992) was that more reliable dispersivity values are needed to
study its scale dependency. A forced gradient tracer test can provide such reliable values. Dispersivities in this study are derived on a scale were no highly reliable observations are available.

Dispersivity values of this study and the data set summarised by Gelhar et al. (1992) is presented in figure 8.1. An increase with scale was found on all field sites. This increase is dependent of the type of sediments being the largest where heterogeneity is also the largest. Here, this is on the Zevergem test site. The difference in heterogeneity was quantified by means of variograms using the natural gamma logs.

Figure 8.1 Dispersivity values derived with this study and the data set summarised by Gelhar et al. (1992). Longitudinal dispersivity used in the regional models of the Stalhille channel ridge (Stalhille CR) and the Westhoek nature reserve (Westhoek NR) are also indicated.

Figure 8.1 also shows the longitudinal dispersivities which were used in the regional models in the second part of this dissertation. It is quite striking that these values are small in comparison with the other data. Groundwater flow simulations in the Belgian coastal plain systematically point to such small values. This is also the case in the Netherlands. Partly, this is due to the detailed water quality observations which are available. Moreover sharp transition zones between fresh and salt water are observed resulting in small dispersivities. Further, the difference is due to inherent model characteristics. When regional models cover relatively small areas (order of kilometres), dimensions of grid cells are also small (order of metres to hectometres). When in addition the hydrogeological situation of the area is well known, this can be implemented quite realistically in the model. The calculated flow will then approximate the real flow relatively accurately. End result is that the dispersivities needed to calculate solute transport will be small. When large grid cells are used (several hundreds of metres) natural occurring variation of hydraulic conductivity in this cells is averaged. Groundwater flow is simulated less accurately and larger dispersivities are needed to simulate solute transport. The same is also the case when not many observations (soft and hard data) are available to construct the model. The lack of knowledge about variations in parameter values is countered by a larger dispersivity value in the model. When in an ideal case the variation of hydraulic and solute transport parameters would be completely known, then solute transport could be simulated using only advection. Dispersivity must in this context thus be seen as a safety net for our limited knowledge of the model domain. It illustrates also that parameter values must be evaluated in the context of the model.
8.2.7 Influence of heterogeneity on pumping test results

Dispersivity and heterogeneity are closely related and this has its consequences for tests aiming to derive dispersivity. The influence of heterogeneity on pumping test results is less studied. Here this influence was studied by simulating pumping tests in heterogeneous aquifers. Drawdowns were calculated in fictive observation wells. These were then interpreted with the inverse model of HYDRA IDEN. Pumping tests were simulated with RMOQ3D (Lebbe, 1978), a 3D groundwater flow model. Pumping tests were simulated in a Theis type of aquifer. Two impervious layers surround one pervious layer. The hydraulic conductivity varies laterally in the pervious layer. A sequential gaussian simulation procedure was used to generate heterogeneous hydraulic conductivity fields, by assuming that \( \ln(K_h) \) is a random function characterised by a spherical variogram. The mean hydraulic conductivity was the same for all simulations but the sill and the correlation length was altered.

Calculations showed that the average hydraulic conductivity is derived with a pumping test in relatively homogeneous aquifers (\( \sigma^2_{\ln(K_h)}<0.5 \)). This level of heterogeneity is found in many groundwater reservoirs indicating that pumping tests are well capable to derive the average hydraulic conductivity of layers.

A different situation arises with larger heterogeneities (\( \sigma^2_{\ln(K_h)}>1.0 \)). In the case of a small correlation length and a large variance, the derived conductivity is larger than the average layer value. This conductivity increases with the variance. Most probably, pathways of high conductivity come into existence. The result of the pumping test is highly weighted by these larger values. When pumping tests are performed on different places in such an aquifer, results can be severely different. The mean value of all these pumping tests will always be larger than the average layer value. This conductivity increases with the variance. Most probably, pathways of high conductivity come into existence. The result of the pumping test is highly weighted by these larger values. When pumping tests are performed on different places in such an aquifer, results can be severely different. The average value of all these pumping tests, however, will always be more or less the same value as the average layer conductivity.

When one observation well is used, the observations can always be matched perfectly by the calculations. Consequence is that one gets the impression that an average conductivity value is derived very reliable for this layer. Depending on the level of heterogeneity this value can be very different as an observation well at another distance from the pumping well is used. If more than one observation well is used the best calculated drawdown values for all these wells must be found. This means that an important difference between observed and calculated drawdowns can exist for one or more observation wells. These differences can be used as a qualitative estimate for the aquifer’s heterogeneity. This information is lost when only one observation well is used.

8.2.8 Push-pull test

As was the case for pumping and tracer tests, we argue to perform field tests to study chemical and microbiological processes and to derive its parameters. A push-pull test is an interesting example of such a test. Therefore, water marked with a conservative and one or more reactive tracers is injected in the groundwater reservoir. Then water is extracted from this well with a constant discharge rate. Water samples are taken with regular time intervals. Comparison between the concentrations of the conservative, non-conservative tracer(s) and possible reaction products is used to study the chemical and microbiological reactions. This can also be quantified in a first-order reaction rate coefficient (Haggerty et al, 1998).

A push-pull test was performed at the Houtave test site. Water was injected in a sand layer containing organic material, situated just below a peat layer. Bromide was used as a conservative tracer, nitrate and dissolved oxygen as a reactive tracer. Aerobic respiration or the oxidation of organic material with
oxygen and nitrate reduction were observed and first-order reaction rate coefficients for these reactions were calculated.

8.3 Applications of parameter identification tests

Reliable parameter values are needed in many applications in hydrogeology. In the first part of this work a number of tests were described and illustrated which can provide these values. These parameter values are interesting as such because they provide information about the characteristics of porous media. But the main aim of parameter identification tests is to derive parameters, which can be used in practical applications. Here a difference is made between applications on the same scale as on which the parameters are derived and applications on larger scales.

8.3.1 Applications on field scale: groundwater pollution problems

Applications on a field scale are more or less on the same scale as on which the parameters are derived. These parameters can be used directly in the application. Clean up of groundwater contamination is an interesting example. Clean up strategies must be studied and planned well beforehand. Knowledge of relevant parameters to simulate the problem is thus necessary.

The Tessenderlo test site is contaminated with 1,2-dichloroethane (1,2-DCA), a carcinogenic and very difficult biodegradable product. Recently, a bacteria *Desulfitobacterium dichloroeliminans* strain DCA1 was identified (Wildeman, 2002) at the Laboratory for Microbial Ecology and Technology (LabMET) of Ghent University which is capable to detoxify 1,2-DCA without the formation of toxic products. This new technology was to be used on the Tessenderlo test site by injecting strain DCA1 in the groundwater reservoir. Beforehand, some crucial questions had to be answered. Obviously, hydraulic and solute transport properties of the aquifer were of interest. Therefore, a forced gradient tracer test was performed and interpreted. The detoxifying properties of strain DCA1 were already proofed in the lab. Next step was to proof that strain DCA1 was active in field circumstances. Therefore, a push-pull test was performed showing the detoxification of 1,2-DCA by strain DCA1. Then mobility of strain DCA1 was questioned and a transport test was proposed. In this test, strain DCA1 was injected in the groundwater reservoir and pulled towards a pumping well. In between, an observation well was present to detect the presence of strain DCA1. Results of this test suggest that strain DCA1 is not very mobile.

This case study illustrated the role of parameter identification tests in different steps in the investigation process. Answers on a number of very practical problems can be provided. Results of the tests done on the Tessenderlo test site will be used in the design of a final clean up strategy.

8.3.2 Regional groundwater flow models

The scale on which parameters are used in regional groundwater flow models is larger than the one on which they are derived. This results in a number of difficulties which should be taken into account during modelling. Heterogeneity causes the aforementioned scaling. Additionally, groundwater flow models are characterised by a lot of input but only by few observations. For instance the variation of hydraulic conductivity in the model domain is in most cases only rudimentary known. The modeller must equilibrate this imbalance.

A model protocol is a first aid. This gives a procedure to follow during the modelling exercise. Based on the aims of the model and the available data, the best suitable computer code is selected and a numerical model is constructed. Early model results show which additional observations or data are needed. These are then collected and imported in the model. Thus, modelling is here an iterative
A second important guide for the modeller are a number of guidelines provided by Hill (1998). These guidelines are mainly focused on the calibration by means of inverse modelling but they are also of use for modelling in general. Besides, it is quite difficult to construct a converging inverse regional groundwater flow model.

The guidelines stress the importance of using difference kinds of information as input and during the calibration of models. These can be head measurements, general geological information, sedimentological data, water analyses, borehole measurements, results of pumping tests, results of tracer tests, infiltration data, discharges, etc. The groundwater flow model must thus be seen as a synthesis of all available knowledge of the study area.

The model must be kept as simple as possible. Otherwise relevant processes are threatened to disappear in its complexity. But it can not be made too simple either. Otherwise the relevant processes are not treated fully at all. A balance must be sought. Hence the importance of selecting the right computer code in the model protocol.

Sensitivity analyses are an interesting tool to study interactions between different parameters and between parameters and observations in a model. During a sensitivity analyses one parameter or property of the model (for instance a boundary condition) is altered and its effects on the model results are investigated. It can be used to identify important knowledge gaps. It can for instance be found that the model results are very sensitive to the hydraulic conductivity of layer X. Then this is an important parameter to determine.

The use of these guidelines is illustrated by means of two regional groundwater models in the Belgian coastal plain. Both deal with the evolution of the fresh salt water quality distribution and the factors influencing this.

8.3.3 Case study: Stalhille channel ridge

The Stalhille channel ridge is situated in the Belgian eastern coastal plain. The freatic aquifer is composed of sandy deposits of quaternary age. More clayey sediments and an important peat layer are found in the adjacent areas. The channel ridge is set higher in relief than the adjacent areas. Until its reclamation, the sea had access in the area through a system of tidal channels and gullies. Before the land reclamation the groundwater reservoir was filled with salt water. The land reclamation was finished in the 12th century AD. Afterwards fresh water infiltrated replacing the salt water. Because the area is situated below mean sea level it is heavily drained. This is especially so for the less permeable areas adjacent to the channel ridge. The geology and the history of land reclamation are responsible for a typical distribution of fresh and salt water. A fresh water lens is present below the channel ridge whereas salt water is present in the adjacent areas.

A 2D groundwater flow model was made to study the development of the fresh water lens. Geological information about the study area and its development together with drilling descriptions, borehole measurements, resistivity soundings and water analyses were used. An interesting connection between geology, geomorphology and water quality was illustrated. An additional set of drillings, borehole measurement and a pumping test were performed and water samples were taken. This information was integrated in the model.

The density dependent groundwater flow model MOCDENS3D (Oude Essink, 2001) was used. Water analyses were maximally integrated in the interpretation of the simulations. Different phases of cation exchange where found along a flow line. Evidence of salinization of fresh waters was found below the fresh water lens indicating the complex hydrogeological history of the coastal plain. Sensitivity analyses showed that the drainage levels mainly influence the depth of the fresh water lens. Hydraulic conductivity of the channel ridge influences mainly the duration of the fresh water lens’ formation. The fresh water lens was formed in about 300 years. An ill-planned pumping of its fresh water can
lead to its destruction in a much shorter period, being years to tens of years. The few fresh water supplies that exist in the coastal plain must thus be protected and well managed.

8.3.4 Case study: Westhoek nature reserve

The Westhoek nature reserve is situated on the most western point of the Belgian coast. It is a dune area of about 340 ha in size and it is one of the last unfragmented dune areas along the Belgian coast. A unique distribution of fresh and salt water is present below the adjacent shore. Salt water is found above fresh water in a dynamic equilibrium. Fresh water infiltrates in the dune area and flows partly towards the sea and partly landwards. Salt water infiltrates on the back shore and flows out on the fore shore and under the sea. This forms a salt water lens above the fresh dune water flowing towards the sea.

A lot of research has been done in the past, consisting of drilling campaigns, borehole measurements, head measurements and water quality surveys. This was used, among other things, as input for a number of simulations. Even an inverse model was made. In the last decade, one became aware of the complex interaction between soil, groundwater and the unique flora and fauna of the dune area but also on the shore and in the landward situated low-lying polder area. Additionally, the dune area is the only local groundwater reservoir where fresh water is present and can be exploited. This is done in the dunes neighbouring the nature reserve. The aim of the simulations in this dissertation was to look at the groundwater flow under the sea, shore, dunes and polder area. Especially the influences on water quality distribution and hydraulic head variations were of interest. Influences on different time scale were studied. These are tides, storms, monthly infiltration variation and sea level rise.

A 2D groundwater flow model was made. The density dependent groundwater flow model MOCDENS3D (Oude Essink, 2001) was used. The available data and the results of past simulations were maximally integrated in this new model. First the groundwater flow under the sea, shore, dunes and polders was simulated. Sensitivity analyses showed that the influence of the hydraulic and solute transport parameters on the general water quality distribution is minimal.

Tides are sea level variations on a very small time scale. This results in a cycle of infiltration of salt water during high tide and seepage of it during low tide. This is also visible in the groundwater flow and hydraulic head pattern below the shore and sea. These fluctuations do not result in variations of water quality distribution. The time scale is therefore too short.

A heavy western storm was simulated using tide gauge measurements of the 1953 storm. It shows the influence of it on the hydraulic heads and groundwater flow. An important extra amount of salt water infiltrates on the shore. Part of this flows landwards. Due to its relatively short duration even a major storm as the one of 1953 has no major effect on the distribution of fresh and salt water.

Monthly variations of infiltration influence the hydraulic heads and groundwater flow. Large infiltration during the winter can lead to large heads in the dunes until the next summer. Influence on the water quality distribution is, however, minimal. Small variations can only be observed in the transition zones. As was the case for tides and storms, monthly variations causes fluctuations of hydraulic heads around a long term steady state situation. It is this long term situation which defines the water quality distribution.

Seal level variations alter the boundary conditions of the flow system (the mean sea level). Additionally sea level variations cause effects on a long time scale (tens of years to hundreds of years). This is more or less the same time period needed to develop the general lay-out of the fresh water tongue and salt water lens under the shore. Therefore sea level rise influences the groundwater flow and the water quality distribution importantly. Different scenarios of the reaction of the coastal morphology (natural and man induced developments) on the sea level rise were considered. Depending on the scenario, the salt water lens under the shore can enlarge, shrink or even completely disappear. Even the important fresh water lens under the dunes can disappear.
The simulations showed that a change of the boundary conditions (mean sea level, drainage level infiltration and coastal morphology), can have severe implications on the flow system. Changing one of these conditions must be studied well beforehand. The nature reserve and adjacent shore and polders are too valuable from an ecological point of view but are also the only local supply of fresh drinking water.
Samenvatting

Transport van opgeloste stoffen in heterogene grondwaterreservoirs:

parameteridentificatie en het gebruik ervan in grondwaterverontreinigings- en zoutwaterintrusie-problematiek

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Inleiding

Heel wat praktische problemen waarmee een hydrogeoloog wordt geconfronteerd, hebben te maken met het transport van opgeloste stoffen. Denken we maar aan de verspreiding van schadelijke stoffen in het grondwater, saneringsvraagstukken, zoutwaterintrusies, beschermingszones rond productieputten, enzovoort. Naast een kwalitatieve beschrijving vraagt deze problematiek heel vaak ook kwantitatieve antwoorden.

Modelleren vormt een belangrijke stap in het zoeken naar een goede oplossing voor deze vraagstellingen. De complexiteit van de processen die zich in het grondwaterreservoir afspelen worden daarbij zo goed als het kan in een model afgesteld. Modellen moeten daarom gezien worden als een synthese van de huidige kennis die we hebben i.v.m. een bepaalde vraagstelling, d.i. zowel met betrekking tot de huidige terreinkennis en –gegevens (geologische opbouw, hydrogeologische parameters, boorgatmetingen, waterkwaliteit, etc) als de huidige inzichten in relevante processen (adveactie, dispersie, diffusie, chemische reacties, microbiologie, etc). Een belangrijk doel van een model is daarbij inzicht te verschaffen in de interactie tussen verschillende componenten van het grondwaterreservoir. Het feit dat we de complexiteit van een grondwaterreservoir in getallen kunnen gieten, ermee rekenen en simulaties uitvoeren zorgt immers voor een enorme meerwaarde in de inzichten die we er over hebben.

Modellen vereisen echter heel wat input, zoals een degelijke schematisatie van het grondwaterreservoir gebaseerd op de geologische kennis, randvoorwaarden, modeleigen parameters en heel wat fysische en chemische parameters zoals hydraulische parameters voor de verschillende lagen, opgeloste stoffen transport parameters, infiltratie, etc. De observaties waarop deze parameters zijn gebaseerd en/of die gebruikt worden om het model te ijken zijn echter beperkt in aantal. Dit leidt tot twee belangrijke moeilijkheden waarmee de modeleerder wordt geconfronteerd:

- Er zijn betrouwbare parameterwaarden nodig, in de eerste plaats voor de doorlatbaarheden van verschillende lagen maar ook voor de specifiek elastische berging, bergingscoëfficiënt nabij de watertafel, dispersiviteit, porositeit, retardatiefactoren, vervalsnellen, enz. Heel vaak zijn deze niet aanwezig en moeten ze ingeschat worden. Daardoor wordt een belangrijke onzekerheid in het model ingebouwd. Het is daarom belangrijk dat praktische en goed uitvoerbare veldproeven worden ontworpen om deze parameters op een adequate en betrouwbare manier af te leiden. Het eerste deel van dit werk spits zich dan ook hierop toe. Een combinatie van een pomproef en een merkproef wordt voorgesteld om hydraulische en opgeloste stoffen transport parameters gezamenlijk af te leiden. Dit wordt vanuit theoretisch standpunt bekeken en geïllustreerd met drie
veldproeven. Tenslotte wordt een veldproef beschreven om chemische reactie te bestuderen en coëfficiënten van eerste orde verval af te leiden. Ook dit wordt met een praktisch voorbeeld geïllustreerd.

- Waarden voor parameters die men zelf heeft afgeleid of die in de literatuur te vinden zijn, kan men niet zonder een aantal bemerkingen gemaakt te hebben verder gaan gebruiken. Een belangrijke eigenschap van grondwaterreservoirs moet in rekening worden gebracht, namelijk de heterogeniteit. Grondwaterreservoirs in sedimentaire gesteenten zijn typisch opgebouwd uit lagen elk met hun sedimentologische eigenschappen. Deze eigenschappen variëren in verschillende mate binnen een bepaalde laag. Een hydraulische doorlaatbaarheid die men op locatie x heeft gemeten kan in meer of mindere mate gaan afwijken van deze gemeten op locatie y, hoewel het dezelfde laag betreft. Dus de heterogeniteit heeft als gevolg dat parameterwaarden kunnen variëren naargelang de plaats waar ze bepaald worden. De mate van variatie is afhankelijk van de mate van heterogeniteit. We zijn nooit in staat om deze ruimtelijke verdeling van parameterwaarden exact af te leiden. Dit moet zodoende opgevangen worden in een model. Een tweede gevolg van heterogeniteit is de opschalingsproblematiek. Parameterwaarden zijn afhankelijk van de schaal waarop ze gemeten worden. Dit is vooraal dispersiveiteit en in mindere mate voor de hydraulische doorlaatbaarheid een goed gekend verschijnsel. Dispersiviteit neemt toe in functie van de schaal waarop ze gemeten wordt.

Er wordt hier, wat betreft de toepassing van hydraulische parameters, dan ook een onderscheid gemaakt op basis van de schaal waarop ze worden toegepast. De toepassing kan op de dezelfde schaal zijn als waarop ze zijn afgeleid. In heel wat saneringstoepassingen is dit bijvoorbeeld het geval. De relevante parameters worden afgeleid op het bewuste terrein en op min of meer dezelfde schaal als de sanering. In regionale grondwaterstromingsmodellen is het gebied waarop de parameter toegepast wordt bijna altijd groter dan de schaal waarop ze is afgeleid.

In het tweede deel van dit werk wordt geïllustreerd hoe hydraulische parameters maximaal samen met andere relevante gegevens kunnen verwerkt worden in een grondwaterstromingsmodel. Een voorbeeld in kader van het opstellen van een saneringsstrategie en twee voorbeelden van regionale modellen wordt aangehaald. De bedoeling van deze laatste is om een inzicht te krijgen in de gedragingen van de grondwaterstroming en het opgeloste stoffen transport.

Identificatie van parameters

Merkerproef met een opgelegde gradiënt


Daarom wordt hier geargumenteerd voor degelijke veldproeven. Dit heeft meerdere voordelen. Eerst en vooral wordt de grondwaterstroming en het opgeloste stoffen transport bestudeerd zoals ze onder veldomstandigheden voorkomen en worden parameters bepaald op relatief grote volumes sedimenten.
De schaal van de proef (zowel ruimtelijk als in de tijd) is tevens niet te groot zodat randvoorwaarden min of meer gekend zijn en in de hand gehouden worden. Twee belangrijke categorieën van proeven komen dan in aanmerking: pompproeven en merkerproeven.

Tijdens een pompproef wordt op een goed doorlatende laag gepompt en de verlaging wordt in deze en in verschillende andere lagen gemeten. Horizontale en verticale hydraulische doorlaatbaarheden, specifiek elastische bergingen en bergingscoëfficiënt nabij de watertafel kunnen zo worden afgeleid. Deze waarden zijn echter gemiddelden voor een bepaalde laag. Met het in dit werk gebruikte softwarepakket HYPARIDEN (Lebbe, 1999) kan de gelaagde heterogeniteit in rekening gebracht worden. Het levert geen of weinig informatie op i.v.m. de laterale variaties in doorlaatbaarheid of de verticale variaties op kleine schaal.

Tijdens een merkerproef op veldschaal wordt een merker geïnjecteerd in het grondwaterreservoir en de verspreiding hiervan wordt bestudeerd. Dit levert een waarde op voor de longitudinale dispersiviteit of de verticale dispersiviteit op. Daarom wordt getracht de voordelen van beide testen te combineren en de nadelen te elimineren in een merkerproef met een opgelegde gradiënt waarbij zowel verlagingen als concentraties worden geobserveerd. Een merkerproef met een opgelegde gradiënt bestaat uit twee stappen. Eerst wordt de merker in het grondwaterreservoir geïnjecteerd. Vervolgens wordt gestart met het pompen op een tweede put. De merker zal daardoor naar deze pompput toe bewegen en dit wordt gevolgd door middel van een aantal observatieputten tussen de pompput en de injectieput. De afstand tussen de injectie- en pompput is tussen de 5 en 10 meter. Zowel metingen van verlagingen als van concentraties worden verricht. Op een dergelijke manier kunnen zowel de hydraulische als de opgeloste stoffen transport parameters gezamenlijk afgeleid worden. Door met twee gegevenssets te werken worden de parameters tevens met een grotere nauwkeurigheid bepaald.

Daarom wordt geacht de voordelen van beide testen te combineren en de nadelen te elimineren in een merkerproef met een opgelegde gradiënt waarbij zowel verlagingen als concentraties worden geobserveerd. Een merkerproef met een opgelegde gradiënt bestaat uit twee stappen. Eerst wordt de merker in het grondwaterreservoir geïnjecteerd. Vervolgens wordt gestart met het pompen op een tweede put. De merker zal daardoor naar deze pompput toe bewegen en dit wordt gevolgd door middel van een aantal observatieputten tussen de pompput en de injectieput. De afstand tussen de injectie- en pompput is tussen de 5 en 10 meter. Zowel metingen van verlagingen als van concentraties worden verricht. Op een dergelijke manier kunnen zowel de hydraulische als de opgeloste stoffen transport parameters gezamenlijk afgeleid worden. Door met twee gegevenssets te werken worden de parameters tevens met een grotere nauwkeurigheid bepaald.

De waarnemingen van verlagingen en concentraties kunnen gezamenlijk uitgevoerd worden tijdens de pompingsfase van de merkerproef. Anderzijds kunnen deze twee datasets tijdens afzonderlijke stappen verkregen worden. Daartoe wordt eerst een pompproef verricht waarbij verlagingen worden gemeten. Daarna wordt een periode gewacht totdat de waterstanden in de peilbuizen terug hun rustniveau bereikt hebben. In een tweede stap wordt de tracer geïnjecteerd, wordt terug gepompt en worden de concentratieobservaties verricht. Om praktische redenen werd hier voor deze tweede optie gekozen.

**Verzamelen van waarnemingen**

De verlagingen die ontstaan door de pompvormen rechtstreeks gemeten met een druksonde in de observatieputten. De concentratiewaarnemingen worden onrechtstreeks bekomen a.d.h.v. geofysische boorgotmeting. Dit heeft alles te maken met de aard van de merker. Door middel van de merkerproef met een opgelegde gradiënt willen we de advectief en dispersief transport bestuderen zonder dat dit gecompliceerd wordt door eventueel optredende chemische reacties. Daartoe is een conservatieve of niet reagerende merker vereist. Er werd geopteerd om zout water te gebruiken. Dit wordt geïnjecteerd in grondwaterreservoirs met zoet tot brak water. Er is dus een belangrijk geleidbaarheidsverschil tussen de merker en het natuurlijk voorkomende water. Hiervan werd dankbaar gebruik gemaakt. EM39 is een toestel die door middel van een gefocussed elektromagnetische inductiemethode de geleidbaarheid van het poriënwater en de sedimenten rond een niet-geleidende waarnemingsput meet. Dit heeft een aantal voordelen t.o.v. vroegere ‘long normal’ en ‘short normal’ opstellingen om de elektrische resistiviteit in boorgaten te meten. De meting kan immers gebeuren in reeds verbruiste boorgaten. De verticale resolutie van de EM39 is hoog. Er wordt met een diepte-interval van twintig centimeter een meting verricht. Dit levert dus een gedetailleerd verticaal beeld op van de passage van de merker rond de waarnemingsput. Dit is een zeer groot
voordeel in vergelijking met bijvoorbeeld wateranalyses om concentratiewaarnemingen te bekomen. Tenslotte kan de elektrische geleidbaarheid gemeten met de EM39 op eenvoudige wijze omgerekend worden naar concentraties van totaal gehalte aan opgeloste stoffen van het poriënwater. Enkel wanneer de geleidbaarheid van de sedimentmatrix belangrijk wordt, is deze relatie minder ondubbelzinnig.

Interpretatie van de merkerproef met opgelegde gradiënt

De verlagingen worden geïnterpreteerd met HYPARIDEN (Lebbe, 1999), d.i. een programmapakket dat toelaat om enkelvoudige en meervoudige pompproeven te simuleren en te interpreteren. Het is gebouwd rond een 2D axi-symmetrisch numeriek model. Het grondwaterreservoir wordt opgedeeld in een aantal lagen. Elke laag wordt gekarakteriseerd door een waarde voor de horizontale en verticale hydraulische doorlaatbaarheid en de specifiek elastische berging. Gelaagde heterogeniteit of de verticale opeenvolging van lagen, kan zo gedetailleerd in het model ingebracht worden. Ieder laag van het numerieke model is inwendig homogeen. De lagen zijn ondervoorin in een aantal coaxiale ringen rond de pompput. De verlaging ten gevolge van een pomping wordt berekend in het nodaal punt van elke ring. De binnen- en buitenstraal van de ringen vormen een logaritmische reeks. De verlaging wordt zodoende ook zeer nauwkeurig berekend dicht bij de pompput, waar de grootste en sterkst in de tijd variërende verlagingen optreden. Het grondwaterreservoir is bovenaan begrensd door de watertafel die gekarakteriseerd wordt door de bergingscoëfficiënt nabij de watertafel. Als ondergrens wordt een ondoorlatende laag verondersteld.

Flexibiliteit en de nauwkeurigheid van de berekeningen vormen het grote voordeel van numerieke modellen zoals HYPARIDEN. Goed ingeburgerde en veel gebruikte analytische modellen bij de interpretatie van pompproeven hebben dit niet. Bij deze analytische modellen wordt gebruik gemaakt van sterk vereenvoudigd schematisering gebaseerd op een beperkt aantal doorlatende en slecht doorlatende lagen. De grondwaterstroming wordt zodoende minder nauwkeurig weergegeven. Een gevolg is bijvoorbeeld dat de lek, d.i. een hoeveelheid water die vanuit omringende lagen naar de aangepompte laag stroomt, wordt onderschat. Dit heeft als gevolg dat de hydraulische doorlaatbaarheid van de aangepompte laag, afgeleid door middel van een pompproef, wordt overschat.


De interpretatie van verlagingen en concentraties is een iteratief proces. De verlagingen worden eerst geïnterpreteerd met het inverse model in HYPARIDEN en hydraulische parameters worden afgeleid. Vervolgens worden deze resultaten gebruikt om de concentratiewaarnemingen te simuleren in TRACER3D. De opgeloste stoffen transport parameters worden afgeleid en indien nodig worden de hydraulische parameters aangepast. Meestal zijn een aantal dergelijke stappen vereist.

Toepassingen: proefsites te Houtave, Zevergem en Tessenderlo

Een eerste merkerproef met een opgelegde gradiënt werd uitgevoerd op de proefsite te Houtave, gelegen in het oostelijk kustgebied. Bedoeling van de proef was om de werkbaarheid van een merkerproef met opgelegde gradiënt aan te tonen, een gegevensset te verkrijgen om TRACER3D uit te testen en om de voordelen van een dergelijke proef met veldgegevens te staven. Het
Samenvatting

A. Vandenbohede

grondwaterreservoir vertoont hoofdzakelijk een gelaagde heterogeniteit met slecht beperkte laterale variaties op schaal van de proefsite. De merkerproef werd uitgevoerd in quartaire sedimenten.

Een tweede proef werd uitgevoerd op de proefsite te Zevergem, gelegen net ten zuiden van Gent. Op deze plaats betaast de freatisch watervloeiende laag uit rivierafzettingen van de Schelde en de sedimenten vertonen een belangrijke heterogeniteit, zowel gelaagd als laterale heterogeniteit. Bedoeling van deze proef was om het concept van de merkerproef met een opgelegd debiet uit te testen in een heteroegen grondwaterreservoir. Daarbij werd ook gewerkt met twee injectieputten respectievelijk geplaatst links en rechts van de pompput, dit om het volume aan sedimenten die in de proef betrokken wordt te vergroten en de laterale heterogeniteit te onderzoeken.

Een derde proef werd verricht op de proefsite te Tessenderlo in Limburg. Het onderzochte grondwaterreservoir is opgebouwd uit glauconietrijke zanden van tertiair ouderdom. In tegenstelling met de twee voorgaande proeven, die louter wetenschappelijke doelstellingen hadden, moest deze proef een aantal praktische vragen oplossen. De site is namelijk gecontamineerd met 1,2-dichloorethaan (1,2-DCA) en een saneringsstrategie moet ontwikkeld worden. Daartoe diende men het verontreinigde gedeelte van het grondwaterreservoir te karakteriseren voor de grondwaterstroming en het transport van opgeloste stoffen.

Resultaten merkerproeven met opgelegde gradiënt

De proefsite te Houtave toonde de uitvoerbaarheid van de proef aan. Tevens werd aangetoond dat de ontwikkelde software TRACER3D goed in staat is om de merkerproef te simuleren en bijgevolg een handig hulpmiddel is voor de interpretatie ervan. Uiteindelijk werden de horizontale hydraulische doorlaatbaarheden van de aangepompte laag en de onderliggende slecht doorlatende laag, de verticale doorlaatbaarheid van de bovenliggende slecht doorlatende laag, de specifiek elastische berging van de aangepompte laag en de onderliggende slecht doorlatende laag, de effectieve porositeit en de dispersiviteit afgeleid.

De hoge verticale resolutie van de EM39 laat toe om met een interval van twintig centimeter een meting te verrichten. Dit betekent dat om de twintig centimeter een doorbraakcurve voorhanden is. Analyse van deze doorbraakcurves laat toe om kwalitatief een idee te krijgen van de heterogeniteit van het grondwaterreservoir. Dit werd eveneens gedaan voor de ander proefsites.

Vergelijkingen van pompproef- en merkerproefresultaten zijn zeldzaam in de literatuur. De overeenkomst tussen resultaten van beide proeven is daarbij in de meeste gevallen ver te zoeken. De hydraulische doorlaatbaarheid afgeleid met een pommproef is veelal groter dan deze afgeleid met een merkerproef. Dit heeft belangrijke implicaties voor het berekenen van reis- en residentietijden van opgeloste stoffen in het grondwaterreservoir. De pommproef werd in deze gevallen telkens geïnterpreteerd met een analytisch model waarbij o.a. de lek van water vanuit omringende (slecht) doorlatende lagen naar de aangepompte laag wordt verwaarloosd. Dit zorgt er voor dat de hydraulische doorlaatbaarheid van de aangepompte laag te groot wordt geschat. De resultaten van de drie proefsites tonen hier aan dat data van pommproeven en merkerproeven wel degelijk met elkaar in overeenstemming kunnen worden gebracht, mits de pommproef op een juiste manier wordt geïnterpreteerd, namelijk met een model dat de optredende grondwaterstroming naar de pompput nauwkeurig genoeg kan simuleren. Dit werd extra aangetoond a.d.h.v. de data van de proefsite te Houtave. De pommproef werd geïnterpreteerd met behulp van een aantal analytische modellen. Deze leiden allen een te grote hydraulische doorlatendheid af. Wanneer doorbraakcurves met deze te grote waarden worden berekend, leidt dit bijgevolg tot een belangrijke onderschatting van het tijdstip van doorbraak van de merker.

Dit betekent niet dat in grondwaterreservoirs waar belangrijke 3D heterogeniteiten aanwezig zijn of in grondwaterreservoirs bestaande uit vaste gesteenten er toch belangrijke verschillen kunnen optreden tussen pommproef- en merkerproefresultaten. Vooral het gebrek aan gegevens om deze heterogeniteiten op een goede manier in een model weer te geven ligt dan veelal aan de basis van de
verschillen er van uitgaand dat de gegeven goed zijn geïnterpreteerd. Dit is veel minder het geval in hoofdzakelijk gelaagde heterogene sedimenten met een beperkte tot middelmatige laterale heterogeniteit.

Aan de hand van de gegevens in de proefsite te Houtave werd met gevoeligheidsanalyses aangetoond dat de hydraulicische en de opgeloste stoffen transport parameters gezamenlijk kunnen worden afgeleid. Deze parameters worden daarbij met een grotere betrouwbaarheid bepaald dan wanneer enkel concentratie- of verlagingsobservaties worden gebruikt. Evenens werd aangegeven dat de transversale dispersiviteit in dit geval niet kan worden afgeleid, zelfs niet met een put die zijdelings van de lijn injectieput-pompput is geplaatst. In een meer algemeen kader kan men de vraag stellen of een betrouwbare waarde voor de transversale dispersiviteit wel kan worden afgeleid met dergelijke proeven. Dit wordt bevestigd door het zeer beperkt aantal goede waarden die in de literatuur te vinden zijn.

De proefsite te Zevergem bevestigt deze algemene conclusies weliswaar in een meer heterogene grondwaterreservoir. Deze heterogeniteit werd duidelijk onderlingd door het feit dat het gedrag van beide merkerchamers totaal anders was. Dit was te wijten aan variaties van hydraulicische doorlaatbaarheid en longitudinale dispersiviteit, wat dan ook gekwantificeerd is geworden. De voordelen die de gecombineerde interpretatie van concentratie- en verlagingsgegevens biedt, wordt duidelijk geïllustreerd. Aan de hand van de verlangingen was het niet mogelijk om de hydraulicische doorlaatbaarheid van een goed doorlatende laag af te leiden. Dergelijke lagen zijn preferentiële wegen voor opgeloste stoffen transport door hun goede doorlaatbaarheid. Het is dus van belang dat deze goed gekarakteriseerd worden. Het afleiden van deze waarde was wel mogelijk door middel van de combinatie van de beide datasets.

De proefsite te Tessenderlo wordt gekenmerkt door glauconieterijke zanden. Dit betekent dat de geleidbaarheid van de sedimentmatrix niet kan verwaarloosd worden in de relatie tussen EM39 geleidbaarheden en het totale gehalte aan opgeloste stoffen in het poriënwater. Deze matrixgeleidbaarheid werd geschat door middel van EM39 metingen in peilbuizen vóór de injectie van de merker en door te veronderstellen dat de formatiefactor en de poriënwatergeleidbaarheid constant zijn in het grondwaterreservoir.

Een interessante vaststelling bij deze proef is het feit dat er voor de simulatie van de waarnemingen minder water (en dus ook zout) moet geïnjecteerd worden dan er in werkelijk geïnjecteerd is geweest. Er is een verschil van 56%. De verklaring hiervoor ligt meer dan waarschijnlijk in de aard van de sedimenten. De doorbraakcurves vertonen namelijk staartvorming. Er is dus een belangrijke hoeveelheid merker die achterblijft in een staart en die slechts heel traag naar de pompput toe beweegt. Dergelijke staartvorming kan niet met TRACER3D worden gesimuleerd waardoor er minder geïnjecteerd dient te worden voor de simulatie. Verschillende oorzaken voor dergelijke staartvorming zijn mogelijk. De hydraulicische eigenschappen van glauconiet zijn met name goed gekend. Passage van zout water kan de doorlaatbaarheid doen afnemen, vooral in een laag met een goede kationenuitwisselingscapaciteit zoals kleihoudende lagen. Verder onderzoek naar de hydraulicische eigenschappen van glauconiet is dus zeker aan te raden. Verder is de relatie tussen EM39 geleidbaarheid en totaal gehalte aan opgeloste stoffen hier nogal vereenvoudigd berekend. Het is goed mogelijk dat de aannames voor de simulatie te eenvoudig zijn. Verder onderzoek naar de verbanden tussen glauconietygaliteit, matrixgeleidbaarheid, poriënwatergeleidbaarheid, sedimentgeleidbaarheid (zoals va gemeten met EM39) is dan ook op zijn plaats.

Geofysische boorgatmetingen worden telkens gebruikt in de interpretatie van de merkproeven. Deze gegevens worden in de eerste plaats gebruikt om samen met de boorbeschrijvingen een schematisatie te maken van het grondwaterreservoir. Verder geven ze informatie over het kleigehalte van sedimenten en dus over de doorlaatbaarheid. Door boorgatmetingen in verschillende putten van een proefsite uit te voeren, kan een idee verkregen worden over de gelaagde en laterale heterogeniteit van de sedimenten. Deze gegevens worden maximaal gebruikt bij de interpretatie van de merkproef.
Longitudinale dispersiviteit

Gelhar et al. (1992) maakten een synthese van de tot dan toe gepubliceerde dispersiviteitwaarden. Dispersiviteit is een parameter waar zeer moeilijk vat op te krijgen is door de schaalafhankelijkheid. De waarde neemt namelijk toe in functie van de schaal, of beter in functie van de reisweg van de opgeloste stoffen. Vanaf een bepaalde schaal wordt een min of meer constante asymptotische waarde bereikt. Deze afstand en de evolutie van dispersiviteit in functie van afgelegde weg zijn afhankelijk van de aard en eigenschappen van de sedimenten. Een van de besluiten van deze publicatie is dan ook dat er meer betrouwbare waarden voor de dispersivities nodig zijn. Een merkproef met opgelegd debiet is in staat dergelijke betrouwbare resultaten te bekomen zodat de resultaten bekeken worden in het kader van het werk van Gelhar et al. (1992). De resultaten van deze studie zijn trouwens gedaan op een schaal waar geen waarnemingen met een grote betrouwbaarheid voorhanden zijn.

De resultaten bekomen in het kader van dit doctoraatsonderzoek worden in onderstaande figuur voorgesteld samen met de gegevens van Gelhar et al. (1992). Een toename van de longitudinale dispersiviteit met de afgelegde weg van de merker werd op alle drie de proefsites waargenomen. Deze toename is echter duidelijk afhankelijk van het grondwaterreservoir. Dit was het grootst op de proefsite te Zevergem waar de heterogeniteit eveneens het grootst is en het kleinst op de proefsite te Houtave waar de heterogeniteit het kleinst is. Dit verschil in heterogeniteit werd gekwantificeerd a.d.h.v. variograms gebaseerd op de boorgatmetingen van de natuurlijke gamma.

Longitudinale dispersiviteiten afgeleid met merkerproeven met een opgelegde gradiënt bepaald op de proefsites te Houtave, Zevergem en Tessenderlo worden weergegeven samen met een gegevensbestand van Gelhar et al. (1992) afgeleid uit literatuurgegevens. Longitudinale dispersiviteiten gebruikt in de regionale modellen van de Stalhille kreekrug (CR) en het Westhoek natuurreservaat (NR) zijn tevens aangegeven.

Tevens wordt op bovenstaande figuur de longitudinale dispersiviteit aangegeven die gebruikt werd in de regionale grondwaterstromingsmodellen in het tweede gedeelte van dit onderzoek. Opvallend, in vergelijking met de dataset verzameld door Gelhar et al. (1992), zijn de kleine waarden die hiervoor gebruikt werden. Modelleringen in het Belgische kustgebied vereisen systematisch kleine waarden voor de dispersiviteit. Ook in Nederland kent men hetzelfde verschijnsel. Deels is de gedetailleerde kennis van de verspreiding van de waterkwaliteit hiervoor verantwoordelijk. Daarbij worden veelal scherpe overgangen tussen zout en zoet water aangetroffen wat uiteraard kleine dispersiviteiten vereist.
om dit te simuleren. Verder is het verschil in belangrijke mate te wijten aan inherente modelkarakteristieken en is zodoende, tot op zekere hoogte, geen fysisch relevant verschijnsel. Wanneer de grootte van regionale modellen relatief beperkt is (orde van kilometers) dan is dit evenzeer het geval voor de dimensies van de gridcellen (orde van meters tot tientallen meters). Wanneer de (hydro)geologische situatie in het modelleergebied daarbij relatief goed gekend is, kan dit nauwkeurig in een model gebracht worden. De berekende stromingen benaderen dan in goede mate de werkelijkheid. Gevolg is tevens dat ook het opgeloste stoffen transport goed kan berekend worden en dat de dispersiviteiten hiervoor nodig klein zijn. Wanneer er met grote gridcellen gewerkt wordt (honderden meters), wordt de variatie in hydraulische doorlaatbaarheid in deze cel uitgemiddeld. De grondwaterstroming en dus ook het opgeloste stoffen transport wordt zodoende minder nauwkeurig gesimuleerd. Hetzelfde gebeurt wanneer er sowieso weinig gegevens voorhanden zijn i.v.m. de variatie van doorlaatbaarheid in het grondwaterreservoir. Gevolg is dat door de in werkelijkheid aanwezige heterogeniteiten de opgeloste stoffen sterker verspreid worden dan gesimuleerd wordt. Dit wordt in het model opgevangen door een grotere dispersiviteit te gebruiken. Als we in het ideale geval de variatie van hydraulische en opgeloste stoffen transport parameters perfect kennen en kunnen weergeven in numerieke modellen dan zou de verspreiding van een opgeloste stof in het grondwater perfect kunnen gesimuleerd worden met advectief transport. Dispersiviteit kan in dergelijke context gezien worden als een opvangnet voor de onvolledige gegevensset die de modellerder ter beschikking heeft. Het geeft ook aan dat parameterwaarden in de context van het model moeten geëvalueerd worden.

*Invloed van heterogeniteit op pomproefresultaten*

Heterogeniteit beïnvloedt ontegensprekelijk dispersiviteit en de resultaten van merkerproeven die tot doel hebben deze waarden af te leiden. Over de invloed van heterogeniteit op pomproefresultaten is echter minder gekend. Dit werd onderzocht door pomproeven in heterogene Theis type aquifer te simuleren, hierbij verlagingen te berekenen in een aantal fictieve putten en deze verlagingen te interpreteren met HYPARIDEN. Pomproeven werden gesimuleerd met RMOQ3D (Lebbe, 1978), een 3D grondwaterstromingsprogramma. De variatie van de hydraulische doorlaatbaarheid wordt berekend volgens een sferisch variogram. De horizontale hydraulische doorlaatbaarheid varieert daarbij lateraal in de aangepompte laag. De gemiddelde waarde voor de doorlaatbaarheid van de aangepompte laag is daarbij steeds dezelfde. Verschillende combinaties van de variatie van het neperiaans logaritme van de doorlaatbaarheid en de correlatielengte worden bekeken.

Resultaten geven aan dat in weinig heterogene reservoirs ($\sigma_{\ln Kh}^2 < 0.5$) de gemiddelde doorlaatbaarheid van een laag afgeleid wordt. Een groot gedeelte van grondwaterreservoirs in sedimentaire gesteenten, toch wat betreft de situatie in Vlaanderen, beantwoordt hieraan. Dit toont duidelijk aan dat pomproeven in de meeste situaties perfect in staat zijn om de gemiddelde doorlaatbaarheid van een lagen af te leiden.

In het geval van reservoirs met een belangrijke heterogeniteit ($\sigma_{\ln Kh}^2 > 1.0$) is de situatie enigszins anders. Met een kleine correlatielengte en een grote variantie is de afgeleide doorlaatbaarheid groter dan de gemiddelde doorlaatbaarheid van de laag. Deze toename wordt groter met de variantie. Er ontstaan wegen met een grotere doorlaatbaarheid waardoor het grondwater zich beweegt. De doorlaatbaarheid die met een pompproef wordt afgeleid, is dan sterk beïnvloed door deze grotere doorlaatbaarheden. Wanneer er op verschillende plaatsen een pommproef wordt gedaan, kunnen de waarden bij grote varianties sterk van elkaar verschillen. De gemiddelde waarde van deze reeks pomproeven zal altijd groter zijn dan het gemiddelde van de verdeling. Met zowel een grote correlatielengte als een grote variantie kunnen zowel grotere als kleinere waarden dan het laaggemiddelde gevonden worden. De grote correlatielengte heeft immers aanleiding tot grote gebieden met een bepaalde doorlaatbaarheid en deze doorlaatbaarheid wordt dan afgeleid. Wanneer er op verschillende plaatsen een pommproef wordt gedaan, kunnen de waarden bij grote varianties sterk van elkaar verschillen. De gemiddelde waarde van deze reeks pomproeven zal echter het laaggemiddelde benaderen.
Wanneer er slechts één waarnemingsput gebruikt wordt, kunnen de waarnemingen altijd zeer goed gesimuleerd worden. Het gevolg is dat je de indruk krijgt dat de doorlaatbaarheid zeer goed is afgeleid. Naargelang de plaats van deze put kan de doorlaatbaarheid echter sterk veranderen bij grote varianties. Wanneer meerdere waarnemingsputten gebruikt worden, wordt de best passende verlagingen berekend voor alle observaties. Dit betekent dat de berekende verlagingen sterk kunnen afwijken van de waarnemingen voor één van de waarnemingsputten of in mindere mate voor meerdere putten. De afwijkingen kunnen dus gezien worden als een kwalitatieve maat voor de heterogeniteit. Deze extra informatie gaat echter verloren als er slechts één waarnemingsput gebruikt wordt.

**Push-pull proef**

Identiek als bij pomp- en merkerproeven zijn er heel wat argumenten om de chemische en microbiologische reacties die zich afspelen in grondwaterreservoirs in voldemortigheden te bestuderen. Dit is de bedoeling van een push-pull proef. Daarbij wordt een hoeveelheid water gemerkt met een conservatieve merker en één of meerder niet conservatieve merkers in het grondwater geïnjecteerd. Daarna wordt met een constant debiet op deze put gepompt tot een volume anderhalf tot tweemaal het injectievolume is opgepompt. Daarbij worden op reguliere tijdstippen watermonsters genomen. Vergelijking van concentraties van de conservatieve tracer met de concentraties van de ander ionen en kationen toont welke reacties opgetreden zijn. Dit kan gekwantificeerd worden in constanten van eerste orde verval (Haggerty et al, 1998).


**Toepassing van parameteridentificatieproeven**

Voor heel wat toepassingen in hydrogeologie zijn betrouwbare parameterwaarden nodig. In het eerste deel van dit werk werden een aantal proeven aangehaald, ontwikkeld en toegepast die daarvoor gebruikt kunnen worden. Deze waarden vertellen heel wat over de eigenschappen van poreuze middens en zijn zodoende vanuit fundamenteel wetenschappelijk oogpunt interessant. Bedoeling van deze proeven is echter veelal om de resultaten in de praktijk toe te passen. Wat de toepasbaarheid van deze parameters betreft, wordt hier een onderscheid gemaakt op basis van schaal.

**Toepassingen op veldschaal: grondwaterverontreinigingsproblematiek**

De toepassingen kunnen op een veldschaal zijn, d.i. min of meer dezelfde schaal als deze waarop de parameters werden afgeleid. De afgeleide parameters zijn dan eigenlijk direct bruikbaar. Saneringen van gecontamineerde terreinen is hier een interessant voorbeeld van. Gezien de hoge kosten moeten dergelijke saneringen vooraf goed doordacht en gepland worden. Kennis van relevante parameterwaarden, zodat de ernst van het probleem en mogelijke oplossingen kunnen gesimuleerd worden, zijn dan ook noodzakelijk. Parameters worden veelal bepaald op het gecontamineerde terrein zelf en op de schaal van de toepassing.

De proefsite te Tessenderlo vormt een voorbeeld van een dergelijk gecontamineerd terrein. Deze site is gecontamineerd met 1,2-dichloorethaan (1,2-DCA), een kankerverwekkend en zeer moeilijk biodegradeerbaar product. Recent werd echter een bacterie, Desulfitobacterium dichloroeliminans stam DCA1, geïdentificeerd (De Wildeman, 2002) die in staat is om 1,2-DCA af te breken zonder dat
er schadelijke bijproducten worden gevormd. Er werd geopteerd om deze nieuwe technologie toe te passen op de proefsite te Tessenderlo door middel van injectie van stam DCA1 in het grondwaterreservoir. Daartoe moest eerst antwoord worden gezocht op een aantal cruciale vragen. Kennis i.v.m. de hydraulische eigenschappen en opgeloste stoffen transport parameters was vereist. Dit werd bekomen door het uitvoeren van een merkerproef met een opgelegde gradieënt. De activiteit van stam DCA1 was in het labo op overtuigende wijze aangetoond. Volgende stap was het aantonen van stam DCA1 activiteit in het grondwaterreservoir. Daartoe werd een push-pull test uitgevoerd. Resultaten van deze proef tonen duidelijk aan dat stam DCA1 in staat is om 1,2-DCA onder veldomstandigheden af te breken. Tenslotte moest achterhaald worden hoe mobiel stam DCA1 in het grondwaterreservoir is. Daartoe werd een transportproef ontwikkeld. Stam DCA1 werd in het reservoir geïnjecteerd om vervolgens naar een pompput te worden getrokken. Tussen injectie- en pompput was een waarnemingsput aanwezig. Resultaten hiervan zijn niet onduidelijk te interpreteren maar suggereren sterk dat stam DCA1 weinig mobiel is.

Deze case study in Tessenderlo illustreert mooi dat de parameteridentificatieproeven in verschillende stappen van het onderzoek een antwoord op een aantal prangende praktisch vragen kunnen geven. De resultaten hiervan worden in een verder stadium gebruikt om tot een definitieve saneringsstrategie te komen.

Regionale grondwaterstromingsmodellen

In grondwaterstromingsmodellen worden parameters gebruikt op een schaal die meestal groter is dan deze waarop ze worden afgeleid. Heterogeniteit zorgt voor de reeds aangehaalde opschalingsproblematiek. Anderzijds worden grondwaterstromingsmodellen gekenmerkt door het feit dat er heel wat inputgegevens vereist zijn doch dat er slechts weinig van deze gegevens door middel van waarnemingen voorhanden zijn. Zo is bijvoorbeeld de juiste variatie van de doorlaatbaarheid in het modelleergebied op z’n best slechts zeer rudimentair gekend. Dit onevenwicht moet door de modellerder zo goed of zo kwaad als het kan in balans gebracht worden.


Een aantal richtlijnen voor de ijking van modellen (Hill, 1998) zijn een tweede belangrijk werkinstrument. Deze richtlijnen zijn hoofdzakelijk gericht op het ijken met een invers model maar zijn ook voor het voorwaarts modelleren bijzonder nuttig. Convergentie bereiken voor een complex systeem als een regionaal grondwaterstromingsmodel is iets wat niet voor de hand ligt en invers modelleren wordt in de praktijk dan ook weinig toegepast.

Deze richtlijnen geven duidelijk het belang aan van het gebruik van verschillende soorten informatie als input, zijnde stijghoogtemetingen, geologische informatie, sedimentologische data, water analyses, boorgatmetingen, resultaten van pompproeven, resultaten van merkerproeven, infiltratiemetingen, debietsmetingen, etc. Het grondwaterstromingsmodel moet op die manier gezien worden als een synthese van de huidige stand van kennis die aanwezig is over het modelleergebied. Het model moet echter niet complexer gemaakt worden dan nodig om een bepaalde probleemstelling op te lossen, want anders dreigt men de werkelijk relevante processen niet meer te kunnen onderscheiden van de minder belangrijke. Anderzijds mag het model ook niet te eenvoudig zijn. In dat geval bestaat immers het gevaar om de essentiële processen te missen. Er moet dus een evenwicht gezocht worden, vandaar het belang van de keuze van een goede computercode in het modelleerprotocol.

Gevoeligheidsanalyses zijn in staat om meer inzicht in een model bij te brengen. Tijdens een gevoeligheidsanalyse wordt één parameter of eigenschap van het model (vb een randvoorwaarde)
gewijzigd en wordt gekeken wat het effect hiervan is. Dit is een belangrijk instrument om leemten in de kennis van een bepaald gebied te identifieren. Zo kan er bijvoorbeeld achterhaald worden dat de modelresultaten bijzonder gevoelig zijn voor de doorlaatbaarheid van een bepaalde laag. Dan is dit een belangrijke parameter die moet bepaald worden.

Deze richtlijnen worden geïllustreerd aan de hand van twee grondwaterstromingsmodellen in de Belgische kustvlakte. Ze behandelen beide de evolutie van de waterkwaliteit in een grondwaterreservoir gevuld met zoet en zout grondwater en de factoren die deze evolutie beïnvloeden.

**Case study: Stalhille kreekrug**

De Stalhille kreekrug is gelegen in het oostelijke kustgebied. De freatisch watervoerende laag is opgebouwd uit zandige sedimenten van quartaire ouderdom. De aangrenzende gebieden, de zogenoemde poelgronden, bestaan uit meer kleiige sedimenten en er komt een belangrijke veenlaag voor. De kreekrug ligt iets hoger in het reliëf t.o.v. de omgeving. De zee kon tot voor de inpoldering vrij in het gebied doordringen door middel van geulen en kreken. Deze inpoldering was algemeen voltooid in de 12de eeuw AD. Het grondwaterreservoir was voor de inpoldering overwegend gevuld met zout water. Na de inpoldering kan er enkel nog maar zoet regenwater infiltreren en grijpt er dus een vervanging op van het oude zoute zeewater met dit zoete infiltratiewater. Het gebied ligt beneden gemiddeld zeespiegelniveau. Dit betekent dus dat het intensief moet gedraineerd worden. Dat geldt vooral voor de poelgronden die slecht doorlatend zijn en is minder het geval voor de beter doorlatende kreekruggen. De geologische gesteldheid en de historische achtergrond van het gebied zorgen dan ook voor een typische verdeling van zout en zoet water. Onder de poelgronden treft men nog het oudere zoute zeewater aan terwijl er zoetwaterzakken aanwezig zijn onder de kreekruggen. Deze kunnen belangrijke zoetwatervoorraden vormen.

Een 2D model werd gemaakt met de bedoeling om het ontstaan en de evolutie van de zoetwaterzak onder de Stalhille kreekrug te modelleren. Een relatief uitgebreide set aan gegevens was daartoe voorhanden. Allereerst is er een uitgebreide kennis i.v.m. de geologische en recent historische evolutie van het gebied voorhanden. Boorgegevens, boorgatmetingen, elektrische sonderingen en wateranalyses tonen mooi het verband aan tussen geologie, geomorfologie en de waterkwaliteit. Verder zijn een aantal boringen, wateranalyses, boorgatmetingen en pompproeven uitgevoerd in en rond de Stalhille kreekrug om in het model te integreren.


**Case study: Westhoek natuurreservaat**

Het Westhoek natuurreservaat is met z’n 340 ha het grootste stukje onaangeroerde duinen van de Belgische kustvlakte. Het is gelegen in het westelijke kustgebied, palend aan de Frans-Belgische

Er is reeds heel wat onderzoek verricht in het gebied. Dit behelst een uitgebreid veldonderzoek bestaande uit boringen, boorgatmetingen, stijghoogtemetingen en wateranalyses. Op basis daarvan zijn een reeks simulaties met numerieke modellen uitgevoerd. Zowel een aantal voorwaartse modellen als een invers model zijn gemaakt. In de laatste tien jaar is men zich echter meer bewust geworden van de complexe en fragile samenhang tussen bodem, grondwater en de unieke fauna en flora die men in het duingebied maar ook in de polders en op het strand aantreft. Tevens zijn duingebieden de enige mogelijkheid om ter plaatse zout water te winnen, iets wat dan ook gedaan wordt in de aan het natuurreservaat grenzende duingebieden. De doelstelling van deze modellering was dan ook de dynamiek van de grondwaterstroom onder de zee, strand, duinen en aanpalende polders te bekijken. Vooral de invloedsfactoren op de waterkwaliteitsverdeling en de stijghoogteconfiguraties staan centraal. Daarbij worden factoren die op verschillende tijdschalen werkzaam zijn bekeken, namelijk invloed van getijden, zware stormen, maandelijkse variaties in infiltratie en zeespiegelwijzingen.

Het 3D dichtheidsafhankelijk grondwaterstromingsmodel MOCDENS3D (Oude Essink, 2001) werd toegepast. Een 2D model werd gemaakt waarin de kennis die opgedaan werd met vroegere modellen maximaal geïncorporeerd werd. In een eerste stap werd een basismodel gemaakt die de grondwaterstroom onder de zee, strand en duinen simuleert. Daarbij werden een aantal gevoeligheidsanalyses gedaan. Deze tonen aan dat de invloed van hydraulische en opgeloste stoffen transportparameters op het globale beeld van de verdeling van zoet en zout water minimaal is.

Getijden zijn, modellmatig beschouwd, cyclische variaties op een korte tijdschaal van de zeespiegel. Een duidelijke cycli van infiltratie bij hoogwater en uitvloeiing bij laag water is te herkennen op het strand. Dit zet zich verder dieper in het grondwaterreservoir. Getijden zorgen zodoende voor duidelijke variaties in de stijghoogtes in de loop van een cyclus. Deze fluctuaties in de grondwaterstroom zijn echter niet van die aard (gezien de beperkte grootte en de korte tijdschaal) dat de waterkwaliteitsverdeling beïnvloed wordt. Dit is immers afhankelijk van een gemiddelde situatie. De invloed van een zeer zware storm werd gesignaleerd aan de hand van zeespiegelstanden waargenomen tijdens de uitzonderlijke storm van februari 1953. Dit toont de belangrijke invloed hiervan aan op de stijghoogtes en dus ook op de grondwaterstroom. Een belangrijke hoeveelheid zout water infiltreert bijvoorbeeld op het hoogstrand een deel hiervan stroomt onmiddellijk landwaarts. Door de relatief korte tijdspanne van een storm wordt de algemene verdeling van zoet en zout water echter niet beïnvloed.

Maandelijkse neerslagvariaties zorgen samen met enkele andere meteorologische factoren voor een maandelijkse variatie in infiltratie. Dit zorgt in de eerste plaats voor een maandelijkse variatie in het stijghoogtepatroon en in de grondwaterstroom. De invloed van een natte winter kan duren tot de volgende droge zomerperiode. De verdeling van zout en zout water wordt echter minimaal beïnvloed. Enkel in de overgangszones kunnen nu wel kleine evoluties waargenomen worden. De tijdschaal waarop infiltratievariaties optreden is hier, in vergelijking met getijden en stormen, wel lang genoeg voor. De infiltratievariaties zijn echter niet van die grootte-orde of langdurig genoeg om een blijvende verandering te veroorzaken. Op termijn schommelt waterkwaliteitsverdeling echter rond een algemeen gemiddelde situatie.

Zeespiegelstijgingen zorgen voor belangrijke veranderingen van de randvoorwaarden, zijnde de gemiddelde zeespiegelstand op een bepaald ogenblik, en zijn werkzaam op een dermate grote tijdschaal, d.i. in dezelfde grootte-orde of groter dan de tijd nodig voor de vorming van de zoutwaterlens en zoetwatertong, dat ze de grondwaterstroom en de waterkwaliteitsverdeling sterk beïnvloeden. Naargelang het scenario kan de zoutwaterlens in omvang afnemen, toenemen of zelfs helemaal verdwijnen. Op termijn kan zelfs de zoetwaterzak onder de duinen sterk in volume afnemen.
De simulaties tonen eveneens aan verandering van de randvoorwaarden (zeespiegelstand, drainageniveaus, morfologie strand) een belangrijke invloed hebben op de grondwaterstroming en de waterkwaliteitsverdeling. Dit is een duidelijke waarschuwing dat veranderingen hiervan, in welke context ook, goed vooraf moeten bekeken worden. Het duingebied en het strand is vanuit ecologisch standpunt en voor de voorziening van drinkwater van te grote waarde.

Referenties


The secret to creativity is knowing how to hide your sources. — Albert Einstein

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