Understanding processes governing water quantity and quality in catchments by using bottom-up and top-down modelling approaches

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Table of Contents

'You have always understood more, my poor friend, than you know.'

C. F. Gauß to A. v. Humboldt in "Measuring the world" by D. Kehlmann

Preface

This postdoctoral thesis and its contributing journal papers resulted from my work as a research scientist over the past eight years, which included a five year period at *Primary Industries Research Victoria* in Tatura, Australia, and my current occupation at the *Water & Earth System Science Competence Cluster* in Tübingen, Germany. The practical orientation of this research was mainly influenced by my Australian experience, whereas the more conceptual and theoretical aspects matured during my time in Tübingen.

I would like to acknowledge my scientific mentors Olaf Cirpka and QJ Wang, who inspired and motivated me. Furthermore, I am grateful to many colleagues who significantly contributed to this work. They are either co-authors of the journal papers contributing to this thesis or they are acknowledged therein. However, I would like to specifically thank Marc Schwientek, Sebastian Gayler, Gunnar Lischeid, Murray Hannah, Thabo Thayalakumaran, Matthew Bethune and Tony Cook. I also thank my students from the University of Tübingen, and in particular Igor Pavlovskiy, for their interest and participation in my research. Finally, I am indebted to my extended family for making this qualification possible.

My postdoctoral thesis is organised as follows. Initially, both the practical context of my research work and the concepts of bottom-up and top-down modelling approaches are introduced. The core of this thesis consists of two chapters. Each chapter summarises selected results from a set of publications following a coherent modelling strategy. The first chapter presents published outcomes from an Australian case study in the Shepparton irrigation region. The second chapter combines one German and one Australian case study from the Ammer and the Barr Creek catchments, respectively. For each case study, I introduce the investigated area and its specific research questions. Concluding remarks are provided separately for each of the chapters.

Tübingen, June 2013

Summary

A better understanding of the dominant hydrological processes in catchments is achievable through a synthesis of top-down and bottom-up modelling approaches, which represent the two fundamental approaches in hydrological sciences. In spite of several calls for a synthesis over the last three decades, this topic has been insufficiently addressed using concrete catchment studies. In this postdoctoral thesis, both bottom-up and top-down modelling approaches were applied in a total of three case studies. These investigations focussed on key processes driving water quantity as well as selected aspects of water quality.

Following the introduction, in chapter two, I present results from a number of studies that applied a bottom-up modelling strategy to obtain a process representation of deep percolation in the Shepparton irrigation region in south-eastern Australia. Deep percolation is a key process in this region controlling both the efficient use of irrigation water and salinity issues. From a lysimeter experiment, we developed an effective model of deep percolation [*Bethune, Selle and Wang*, 2008; *Selle and Muttil*, 2011], which was positively benchmarked against models based on Richards' equation [*Selle, Minasny, Chandra, Thayalakumaran and Bethune*, 2011]. The effective model had only two model parameters representing key soil properties governing deep percolation in the lysimeter experiment. The regionalisation problem was simplified because only these two soil parameters needed to be estimated for the Shepparton irrigation region. However, we found that the most important model parameter, i.e. the final infiltration rate of the permeability restricting subsoil, could only be poorly regionalised. This model parameter was unrelated to basic soil properties that were also readily available from soil maps [*Selle, Wang and Mehta*, 2011]. Furthermore, the extent to which our effective model of deep percolation may be representative for regional scale processes remained uncertain. Overall, the studies presented in chapter two of this work demonstrated a number of challenges of bottom-up modelling strategies.

In chapter three, bottom-up and top-down modelling approaches were synthesised for two different catchment studies. The first study [*Selle, Thayalakumaran and Morris*, 2010; *Selle and Hannah*, 2010; *Githui, Selle and Thayalakumaran*, 2012] investigated salt mobilisation processes from the irrigated Barr Creek catchment in south-eastern Australia, which is a major contributor of salt to the Murray River. From a combined application of bottom-up and top-down approaches, complementary insights into the dominant processes driving the export of salt from the catchment were obtained under different climatic conditions. The second case study examined processes governing selected aspects of groundwater quality for the Ammer catchment in south-western Germany [*Selle, Rink and Kolditz*, 2013; *Selle, Schwientek and Lischeid*, 2013; *Pavlovskiy and Selle*, submitted]. The Ammer catchment is extensively used for drinking-water production from a karstified carbonate aquifer. We initially applied top-down approaches to obtain a conceptual model of water flow and solute transport in the carbonate aquifer. This conceptual model was subsequently refined using a spatially explicit groundwater flow model. In conclusion of chapter three, both case studies demonstrated that it is possible to obtain a relatively reliable and detailed understanding of flow and transport processes from a combination of top-down and bottom-up modelling approaches.

Publications

Bethune, M.G., B. Selle, and Q.J. Wang (2008), Understanding and predicting deep percolation under surface irrigation, *Water Resources Research*, 44, W12430. (**Appendix A**)

Selle, B. and M. Hannah (2010), A bootstrap approach to assess parameter uncertainty in simple catchment models, *Environmental Modelling & Software*, 25, 919-926. (**Appendix B**)

Selle, B., T. Thayalakumaran and M. Morris (2010), Understanding salt mobilization from an irrigated catchment in south-eastern Australia, *Hydrological Processes*, 24, 3307-3321. (**Appendix C**)

Selle, B., B. Minasny, S. Chandra, T. Thayalakumaran and M.G. Bethune (2011), Applicability of Richards' equation models to predict deep percolation under surface irrigation, *Geoderma*, 160, 569-578. (**Appendix D**)

Selle, B. and N. Muttil (2011), Testing the structure of a hydrological model using Genetic Programming, *Journal of Hydrology*, 397, 1-9. (**Appendix E**)

Selle, B., Q.J. Wang and B. Mehta (2011), Relationship between hydraulic and basic properties for irrigated soils in southeast Australia, *Journal of Plant Nutrition and Soil Science*, 174, 81-92. (**Appendix F**)

Githui, F., B. Selle and T. Thayalakumaran (2012): Recharge estimation using remotely sensed evapotranspiration in an irrigated catchment in southeast Australia, *Hydrological Processes*, 26, 1379-1389. (**Appendix G**)

Selle, B., K. Rink and O. Kolditz (2013), Recharge and discharge controls on groundwater travel times and flow paths to production wells for the Ammer catchment in southwestern Germany, *Environmental Earth Sciences*, 69, 443-452, EES Topical Issue "Catchment Research". (**Appendix H**)

Selle, B., M. Schwientek and G. Lischeid (2013), Understanding processes governing water quality in catchments using principal component scores, *Journal of Hydrology*, 486, 31-38. (**Appendix I**)

Pavlovskiy, I. and B. Selle (submitted), An integrated approach to delineate capture zones of wells and associated transit times of water for karstified and fractured aquifer systems, *Grundwasser*, Thematic Issue "Karst Hydrogeology". (**Appendix J**).

My contribution to each publication

Appendix A - *Bethune, M.G., B. Selle, and Q.J. Wang (2008), Understanding and predicting deep percolation under surface irrigation, Water Resources Research, 44, W12430.*

The lysimeter experiment in Tatura, which provided the data for this publication, was designed by Matthew Bethune and QJ Wang. I developed the conceptual model of deep percolation based on the lysimeter data with inputs from Matthew and QJ. I conducted all data analyses and computations, and I also wrote the paper.

Appendix B - *Selle, B. and M. Hannah (2010), A bootstrap approach to assess parameter uncertainty in simple catchment models, Environmental Modelling & Software, 25, 919-926.*

The bootstrap approach presented in this paper was co-developed by Murray Hannah and me. I wrote the computer codes, processed the data and performed all computations. Murray and I co-wrote the paper.

Appendix C - *Selle, B., T. Thayalakumaran and M. Morris (2010), Understanding salt mobilization from an irrigated catchment in south-eastern Australia, Hydrological Processes, 24, 3307-3321*

I designed and conducted the study including data analysis, model development and computations. I wrote the paper with inputs from Thabo Thayalakumaran and Mike Morris.

Appendix D - *Selle, B., B. Minasny, S. Chandra, T. Thayalakumaran and M.G. Bethune (2011), Applicability of Richards' equation models to predict deep percolation under surface irrigation, Geoderma, 160, 569-578.*

I had the idea for this study together with Budiman Minasny. I designed and conducted the study. The adequacy test used in this study was suggested by Subhash Chandra. I wrote the paper with inputs from all other co-authors.

Appendix E - *Selle, B. and N. Muttil (2011), Testing the structure of a hydrological model using Genetic Programming, Journal of Hydrology, 397, 1-9.*

I had the idea for this publication and designed the study. Nitin Muttil performed the computations using Genetic Programming; and we interpreted the outcomes together. We co-wrote the paper.

Appendix F - *Selle, B., Q.J. Wang and B. Mehta (2011), Relationship between hydraulic and basic properties for irrigated soils in southeast Australia, Journal of Plant Nutrition and Soil Science, 174, 81-92.*

QJ Wang and Brijesh Mehta designed and lead the field study, which provided the data for this paper. I analysed the data and wrote the paper with inputs from my co-authors, in particular on the "Material and Methods" part.

Appendix G - *Githui, F., B. Selle and T. Thayalakumaran (2012): Recharge estimation using remotely sensed evapotranspiration in an irrigated catchment in southeast Australia, Hydrological Processes, 26, 1379-1389.*

I developed the idea and the concept for this paper with inputs from Thabo Thayalakumaran. Faith Githui set up the SWAT model and conducted this study with my guidance. Faith and I co-wrote the paper with some inputs from Thabo.

Appendix H - *Selle, B., K. Rink and O. Kolditz (2013), Recharge and discharge controls on groundwater travel times and flow paths to production wells for the Ammer catchment in southwestern Germany, Environmental Earth Sciences, 69, 443-452.*

I designed and conducted this study and wrote the paper. Karsten Rink and Olaf Kolditz helped with different aspects of setting-up the OpenGeoSys model which was used in this study.

Appendix I - *Selle, B., M. Schwientek and G. Lischeid (2013), Understanding processes governing water quality in catchments using principal component scores, Journal of Hydrology, 486, 31-38.*

I designed and conducted this study and wrote the paper. Marc Schwientek and Gunnar Lischeid helped with the interpretation of the results from the principal component analysis and provided inputs to the manuscript writing.

Appendix J - *Pavlovskiy, I. and B. Selle (submitted), An integrated approach to delineate capture zones of wells and associated transit times of water for karstified and fractured aquifer systems, Grundwasser.*

I had the idea for this study. Igor Pavlovskiy designed and conducted this study as a Master thesis under my supervision. I wrote the paper based on Igor's results.

1. Introduction

Fresh water is essential for life but only 2.5 % of all water on earth is fresh water and most of it is stored in polar icecaps and glaciers [*Hornberger et al.*, 1998]. Rainfall on land represents the only source of fresh water that renews regularity [*Postel et al.*, 1996]. The flow of renewable fresh water from the land to the sea is organised in river catchments. A proper management of these catchment water resources requires an understanding of the processes governing its quantity and quality. This understanding could be best achieved by an integration of top-down and bottom-up modelling approaches, which are the two fundamental approaches applied in hydrological sciences.

For bottom up approaches, one typically starts with process models describing local scale flow and transport in particular compartments such as in soils, aquifers and water bodies (Figure 1). To arrive at a catchment scale model, first those local process representations need to be coupled across different compartments [e.g. *Freeze and Harlan*, 1969]. In a second step, regionalisation techniques are applied to obtain model inputs and parameters at catchment scales [e.g. *Götzinger and Bardossy*, 2007]. The bottom-up approach will typically lead to a complex catchment model representing flow and transport processes in a spatially explicit manner.

In contrast, for top-down approaches, catchment scale observations such as river discharges or solute concentrations will be the starting point. From these observations, one initially separates out processes explaining the variability of measurements with a minimum number of assumptions; and these identified processes need to be localised subsequently [*Sivapalan et al.*, 2003]. For many catchment scale applications of either one of the two modelling approach, major assumptions will be involved. This is particularly true for the second step of each modelling paradigm, i.e. the parameterisation of a spatially explicit process model and the localisation of processes coming out of a top-down modelling approach.

The difference between the two paradigms, and in particular the way of thinking associated with it, is characterised by *Savenije* [2009]. He calls the bottom-up approach 'Reductionism', which '... is strongly related to causality, and causality is easier to identify from small to large than in the opposite direction. The operation of piecing together small elements and generating progressively larger elements, which is at the heart of "physically based" hydrological models, may be a more natural operation for the human brain. Thinking in the opposite direction of the causality chain, instead, requires imagination, inspiration, insight, field experience, creativity, ingenuity and skill.' The "opposite direction" is then obviously what I call the top-down approach; and the challenging aspects of it may be slightly overemphasised by *Savenije* [2009]. Useful application of both bottom-up and top-down approaches to real catchments require, e.g., field experience. An interesting historical perspective on the two fundamental approaches used in hydrological sciences provides *Young* [2013]. The bottom-up approach, which he calls "hypothetico-deductive", is in his opinion 'largely a creature of the twentieth century and is linked strongly with laboratory science and the ability to carry out planned experimentation'. He further explains that, before the twentieth century, the alternative top-down approach, which he calls "hypothetico-inductive", was typically applied for scientific investigations.

For these, a model was inferred directly from observations of the system under study without any prior hypotheses about its behaviour.

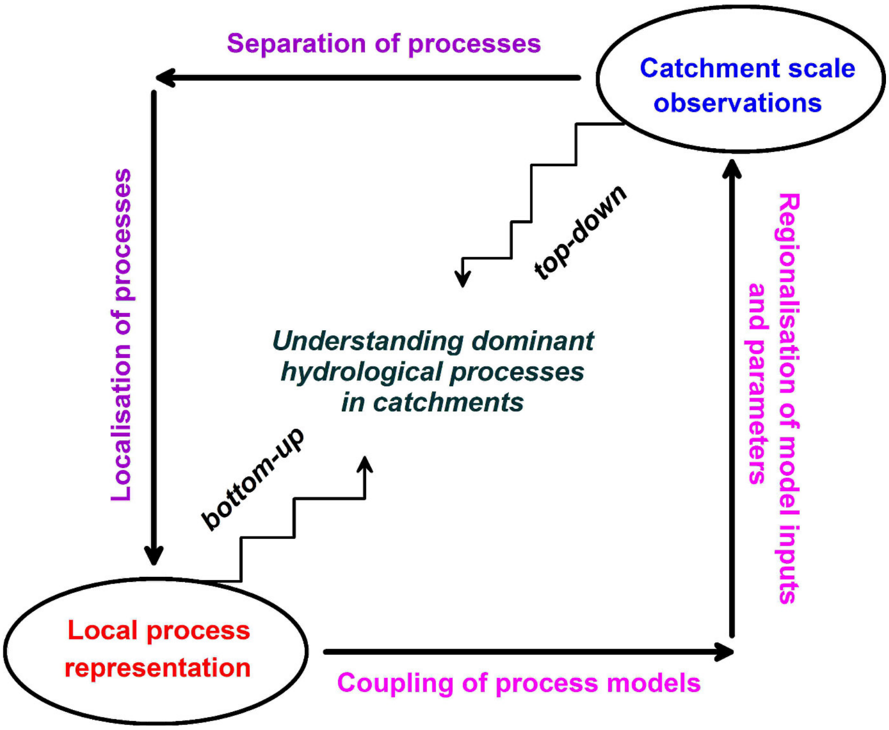

Figure 1: *Integration of top-down and bottom-up modelling approaches.*

The idea of a synthesis or integration of top-down and bottom-up approaches has been around in hydrological sciences for a few decades now. Already *Klemeš* [1983] in his seminal paper Conceptualization and Scale in Hydrology stated that '… the most promising route to significant new discoveries in hydrology is to combine the upward and downward search based on the existing facts and knowledge as well as on imagination and intuition…'. Or as *Dooge* [1986] put it a little later: "… hydrology at the present time draws both on a microscale approach based on continuum mechanics and on a macroscale approach based on the statistical study of large aggregates. Neither approach is entirely appropriate to catchment hydrology, which involves systems intermediate in size between the local scale of hydrologic physics and the global scale of a major geographical region' and he further points out that '…the laws of catchment hydrology are to be based on a parameterisation of the microscale nonlinear equations of physical hydrology or on a disaggregation of long-term macroscale equilibrium relationships or on a combination of both these approaches'.

Recently, *Sivapalan et al.* [2011] called for a synthesis of "Newtonian" and "Darwinian" approaches in hydrology, which, in my opinion, conveys a similar idea, i.e. to iteratively zoom in and out when studying catchment hydrology to better understand the relevant processes and structures. However, I believe that both the scale and scope of the call by *Sivapalan et al.* [2011] are somewhat different to what I actually present in my postdoctoral thesis. From my interpretation, they seek the organizing principles of dominant hydrological processes and its associated patterns at regional to global scales by a combination of top-down and bottom-up modelling approaches, which they call "Darwinian" and "Newtonian", respectively. The terminology, used by *Sivapalan et al.* [2011], was adapted from *Harte* [2002] who suggested a synthesis of physics-like "Newtonian" and ecology-like "Darwinian" approaches to progress in Earth system sciences.

Although the idea of a synthesis of the two schools of thought in hydrology has been communicated for a long time within the scientific community, applications of this idea to practical case studies hardly exist in the body of literature. More specifically, the two steps required for each modelling approach (Figure 1) are rarely reported for a given system under study, let alone are the two paradigms brought together in a coherent manner. There are - to my knowledge - no practical examples where the two modelling approaches were brought together in a concrete case study. In this postdoctoral thesis, I first present a specific bottom-up strategy to model deep percolation in an irrigation region of south-eastern Australia. Subsequently, the integration of top-down and bottom-up modelling approaches is demonstrated for two different catchment studies. These catchment studies investigated key processes related to water quantity and selected aspects of water quality.

2. A bottom-up modelling strategy

2.1. Deep percolation in the Shepparton irrigation region, south-eastern Australia

The study area presented in this chapter is the Shepparton irrigation region in the southern Murray-Darling Basin of Australia (Figure 2). The Shepparton irrigation region is a major irrigation region in Australia; and a significant proportion of the surface water resources available in the Murray-Darling Basin is used for irrigation purposes here [*Wang et al.*, 2009].

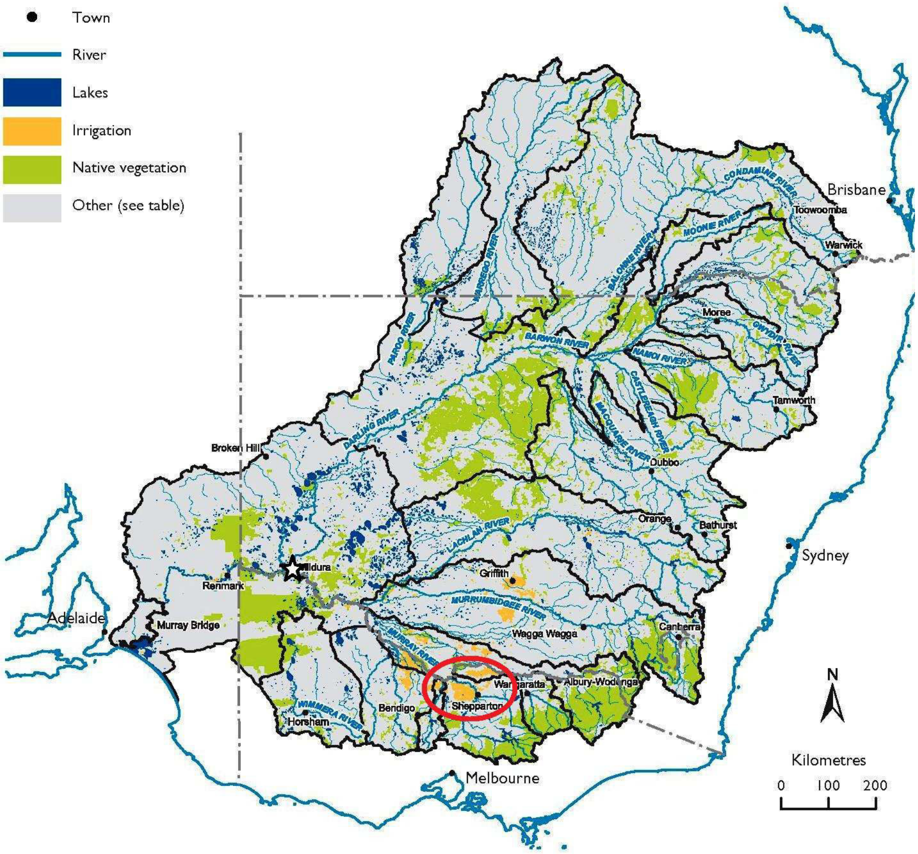

Figure 2: *Landuse across the Murray-Darling Basin of south-eastern Australia [CSIRO, 2008]. Irrigation areas are displayed in orange and the red ellipse indicates the Shepparton irrigation region. Location of Murray River gauging station at Wentworth is indicated by a white star (see Figure 3 for streamflow data).*

The Shepparton irrigation region covers a land area of 5,200 km², of which approximately 3,000 km² are irrigated. The dominant landuse is pasture, which is mainly used as feed for dairy cows. Pasture is usually surface-irrigated, where water is flooded over a graded irrigation bay. Surface irrigation is the most widespread method of irrigation, accounting for about 90% of the total irrigated land. The climate is semiarid, with hot summers. The average annual rainfall is 490 mm, with large variability and slightly higher rainfall in winter. The relief is almost flat. The soil formation in the region is associated with alluvial processes. Most of the soils of the region are layered, locally known as duplex soils. Duplex soils are characterized by relatively shallow topsoils and subsoils with low water permeability.

There are two main factors making the management of irrigation water in the Shepparton irrigation region a difficult task. The first factor is the pronounced temporal variability of rainfall and thus the potential availability of surface water resources for irrigation. This variability is exemplified in a graph of annual stream flows in the Murray River over the last 40 years with remarked changes of relatively wet and dry periods (Figure 3).

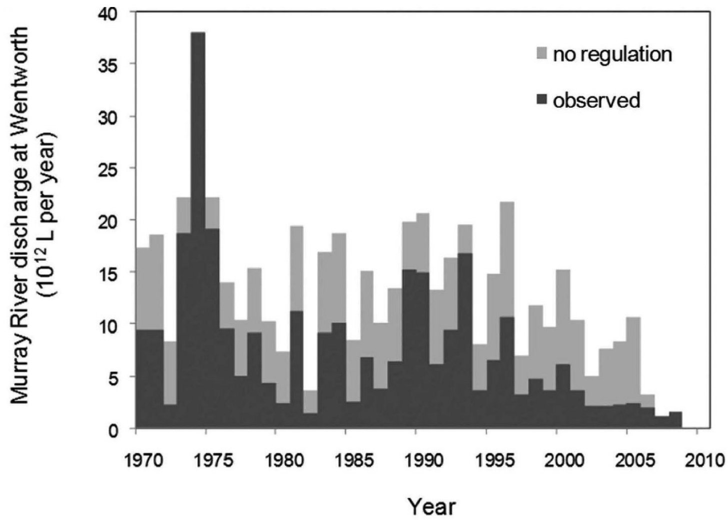

Figure 3: *Variability of annual flow in the Murray River at Wentworth [van Dijk et al., 2013], near the confluence with the Darling River (see Figure 2 for location) as observed (dark grey) and as estimated to have occurred in the absence of river regulation such as impoundment, release and extraction of flows (light grey).*

The other factor is that a significant part of the groundwater system in the basin is extremely salty which is related to salinity issues [*Herczeg et al.*, 1993]. Deep percolation is intimately linked to both of these factors and is therefore a key variable for water management in the region [*Bethune*, 2004]. For below average rainfall periods, deep percolation represents a loss of irrigation water that unproductively percolates below the plant root zones. It also influences sustainable yields for groundwater extraction where groundwater is relatively fresh. Under relatively wet climatic conditions, excessive deep percolation leads to shallow watertables and will cause soil salinity and discharge of saline groundwater into water courses. Salt mobilisation into surface water bodies is particularly relevant if the salt ends up in the Murray River, with serious problems for downstream water users [*Duncan et al.*, 2008].

2.2. Lysimeter experiment and a model of deep percolation

The following section will present selected results from the paper by *Bethune, Selle and Wang* [2008]. Please see this publication in the appendix A for additional or more detailed information.

A lysimeter experiment was conducted in Tatura, south-eastern Australia, to quantify the deep percolation response under surface irrigated pasture to different soil types, depths of the watertable below the ground surface, and ponding times during surface irrigation.

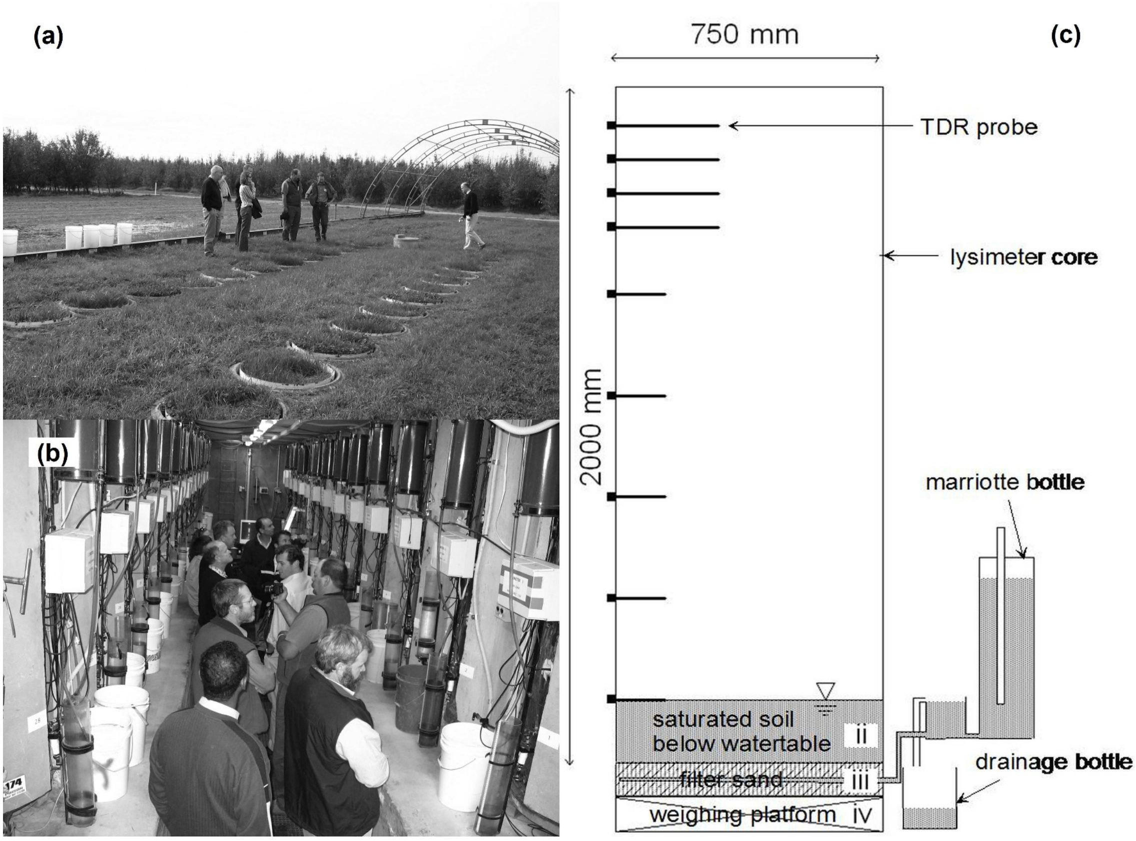

Figure 4: *Lysimeter experiment in Tatura. (a) An aboveground view of the lysimeter facility during an irrigation event; (b) An underground view of the lysimeter facility; (c) A schematic of the lysimeter instrumentation. Depth of the watertable below the ground surface was set by applying a constant water pressure to the base of the lysimeters using Mariotte bottles.*

The experiment aimed at quantifying deep percolation and its main drivers for the dominant landuse and irrigation practise in the Shepparton irrigation region, i.e. surface irrigated pasture. It was thought that, using a controlled experiment, the complex process of deep percolation in the region could be simplified to formulate an effective model of deep percolation. Its process description would concentrate on the important inputs and model parameters, which could also be regionalised. We anticipated that this effective model could be used as a robust estimation tool for recharge processes throughout the Shepparton irrigation region.

During surface irrigation in a real world situation, which the lysimeter was meant to represent, water is flooded over a graded irrigation bay. The ponding time is the interval during which irrigation water will infiltrate at a specified location. It begins when irrigation water first reaches a particular location and ends when the water eventually drains from there. Lysimeters represented 25 undisturbed soil cores of 0.75 m diameter and 2.2 m depth, with 8 soil types varying between sand and heavy clay and fixed depths of the watertable below the ground surface ranging from 0.6 m to 1.8 m (Figure 4). Perennial pasture was established in the cores that were irrigated. An irrigation event consisted of maintaining a pond of water of approximately 7 cm depth on the lysimeter surface for a period of 3, 6, 9 or 12 hours. For each lysimeter, soil moisture was continuously measured using time domain reflectometry (TDR) at different soil depths.

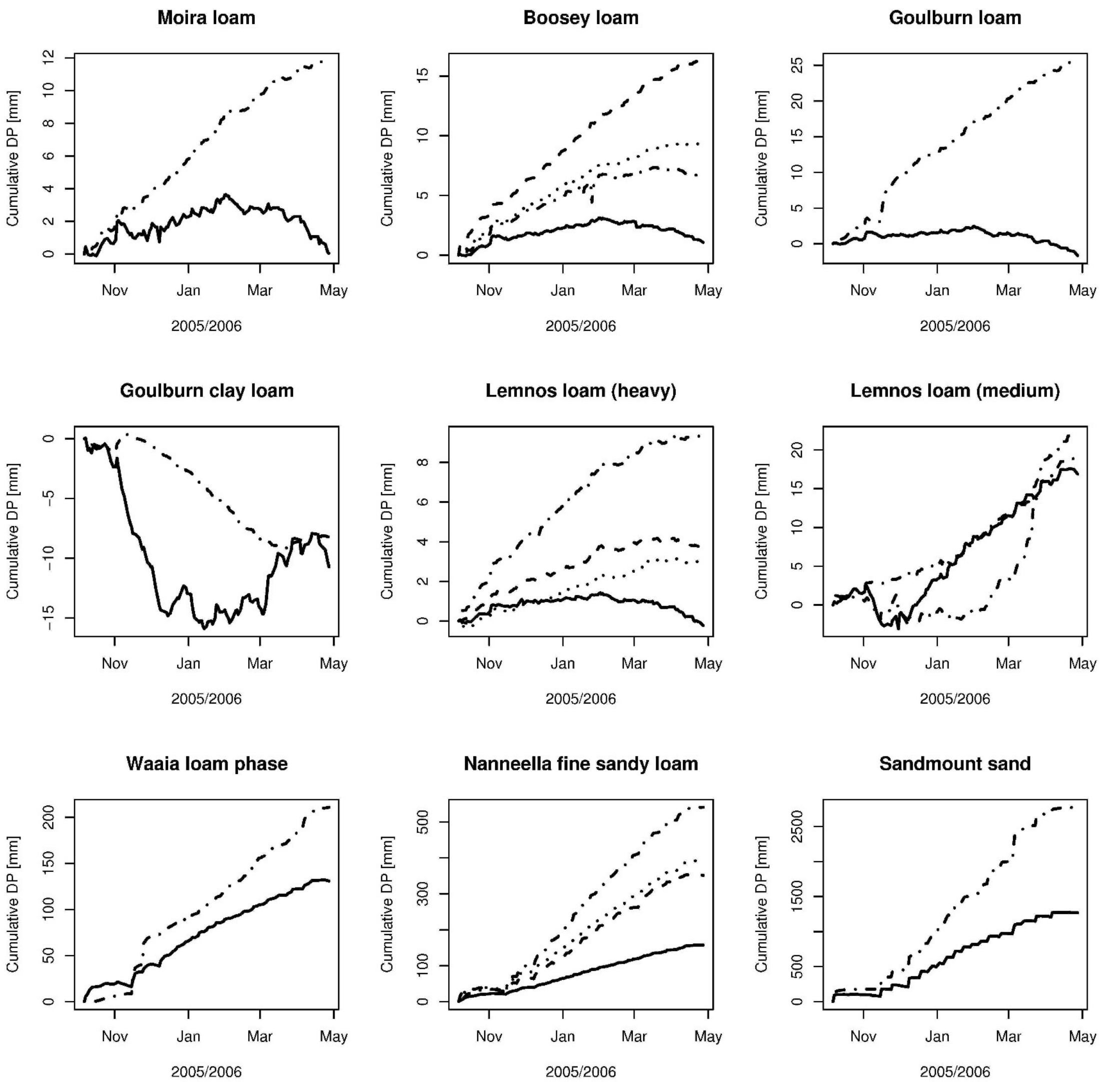

Figure 5: *Measured cumulative deep percolation for all 25 lysimeters in 2005/06. Lysimeter cores with depths of the watertable below the ground surface of (solid lines) 0.6 m, (dashed lines) 0.9 m, (dotted lines) 1.2 m, and (dash-dotted lines) 1.8 m.*

A total of 450 deep percolation events were measured as a result of 18 irrigation events applied to the 25 lysimeters during the 2005/2006 irrigation season. Deep percolation was measured as cumulative amounts of water between two consecutive irrigation events. Temporal variability and magnitudes of measured deep percolation can be seen from Figure 5 showing periods of net drainage and capillary rise.

Three steps were taken to develop an effective model of deep percolation with a minimum number of model parameters and inputs. As a first step, the experimental data was analysed to identify key variables that governed deep percolation. Classification and regression trees (CART) [*Breimann et al.*, 1984] were used for this analysis. The basic idea behind CART, which can be used to solve both regression and classification problems, is to identify increasingly homogeneous configurations of input variables that should lead to increasingly homogenous configurations of response variables. Input variables, potentially driving deep percolation responses, included information that would typically be used in models simulating saturated–unsaturated water flow:

a) The final infiltration rate of the subsoil (i_f) was measured in the field using infiltration rings (350 mm in diameter). As water permeability was mainly restricted by the fine-textured subsoil, it provided information on the effective near-saturated hydraulic conductivity for each of the eight soil types.

b) The soil water stored in the rootzone between saturation and field capacity (DW) is often associated with the amount of water that can drain through the soil during redistribution. For each soil type, soil water retention properties were measured in undisturbed core samples of 73 mm diameter using ceramic suction plates.

c) The lower boundary condition was described by the depth of the watertable below the ground surface (GWD) of each lysimeter core.

d) The upper boundary condition for each irrigation event was characterized by the ponding time (t_o), the daily average rainfall and sum of daily crop evapotranspiration (ET) between two consecutive irrigations.

e) The initial condition was described by the water content in 0.1-m soil depth prior to an irrigation event.

From the CART analysis, the final infiltration rate of the subsoil, the duration of irrigation, and the depth of the watertable below the ground surface were identified as the key variables explaining deep percolation measured at the event scale.

In a second step, two important processes were identified from the observed typical soil moisture responses of the soils to irrigation events (Figure 6). Soil moisture response typically first indicated a percolation phase under steady-state and then under non-steady state conditions, i.e. a redistribution phase.

As a third step, the two dominant processes, i.e. steady-state percolation (SSP) and nonsteady-state percolation ($NSSP$), were parameterised using the key variables identified from the CART analysis to formulate a model of deep percolation (Figure 6). The model of deep percolation (DP) is given by:

$$DP = \left(\underbrace{i_f t_o}_{SSP} + \underbrace{a \frac{DW}{ET} i_f}_{NSSP} \right) f(GWD)\,, \tag{1}$$

where a is an empirical coefficient describing the time-constant percolation rate during redistribution. The term i_f t_o represents the percolation during irrigation (when irrigation water is ponding on the soil surface) assuming steady-state conditions. The ratio DW/ET denotes the time required for evapotranspiration to utilize DW. Both SSP and $NSSP$ are affected by a factor representing the watertable influence:

$$f(GWD) = \tanh\left(0.55 \frac{GWD}{GWD_0}\right), \tag{2}$$

where GWD_0 is defined as the half depth of watertable influence (analogous to the half-life concept in radioactive decay), i.e., when GWD=GWD_0, the reduction factor f is tanh(0.55), which is 0.5. The reduction factor becomes zero for watertables at the soil surface (no deep percolation) and approaches unity for deep watertables (free draining conditions, no capillary rise). For the soils investigated, GWD_0 was estimated to be 1 m.

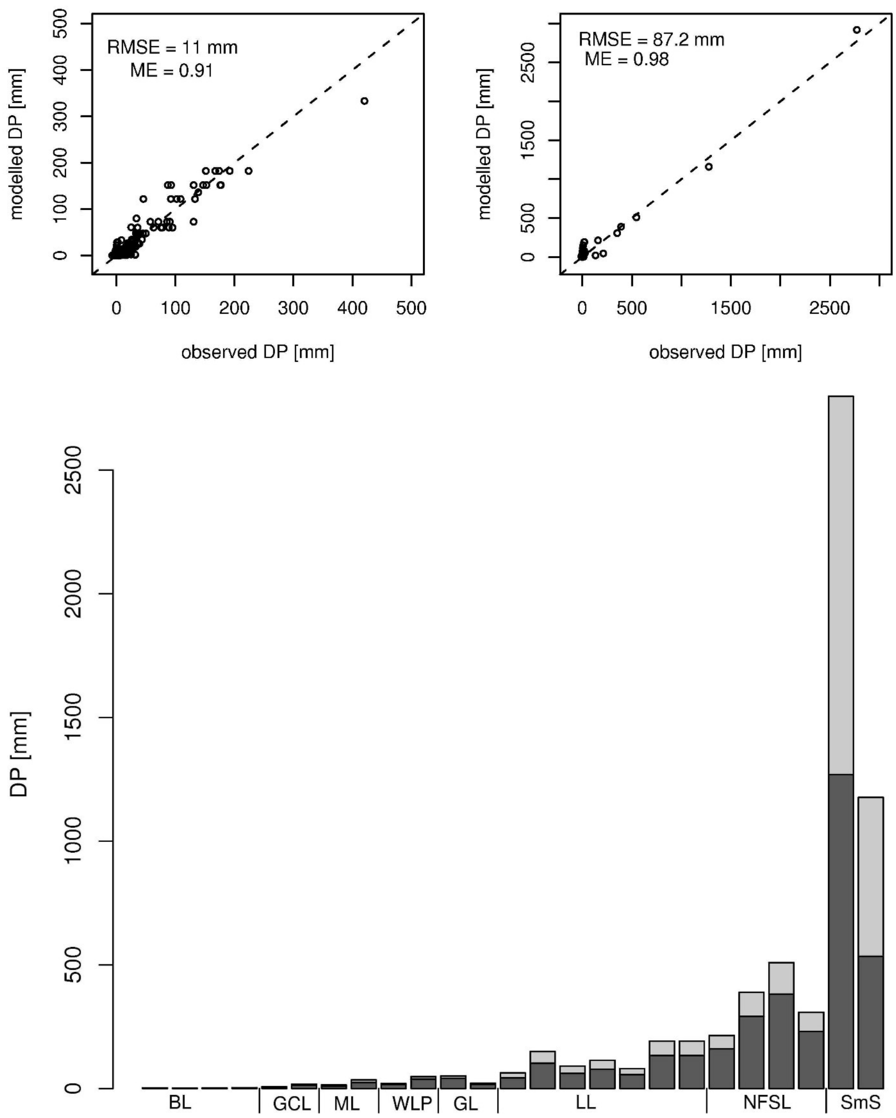

Figure 6: *Deep percolation measured in the lysimeter experiment versus model predictions at the scale of single irrigation events (top left) and at a seasonal scale (top right). Performance of models was assessed using the Nash-Sutcliffe model efficiency (ME) and the root-mean-square error (RMSE). Bottom graph displays seasonal deep percolation in 2005/06 for different lysimeters and contributions from steady-state (dark grey bars) and nonsteady-state percolation (light grey bars) estimated using our model of deep percolation.*

Our model of deep percolation predicted the lysimeter data well both at the scale of a single irrigation event and also at a seasonal scale (Figure 6 top). We found, using our model, that steady-state percolation during irrigation was the dominant process contributing to deep percolation for most of the studied soils. Nonsteady-state percolation (redistribution) was also important for some of the sandier soil types (Figure 6 bottom).

2.3. Testing and benchmarking the model of deep percolation

Our model of deep percolation, given by equations (1) and (2), was benchmarked against a model based on Richards' equation [*Selle, Minasny, Chandra, Thayalakumaran and Bethune*, 2011]. The model structure of our model was also tested using Genetic Programming [*Selle and Muttil*, 2011]. In the following section, selected results from the above mentioned journal papers are presented; and they should also be consulted in the appendices D and E for additional or more detailed information.

From a test of Richards' equation models for the lysimeter data, we found that they had an inadequate model structure for representing deep percolation under surface irrigation as preferential infiltration was not accounted for. Preferential infiltration can probably not be avoided under surface irrigation due to ponding conditions. In contrast to Richards' equation models, our simpler model adequately predicted deep percolation. Note that the rootzone in our model was represented as a single bucket that fills instantaneously when irrigation water is applied and then overspills controlled by key soil properties, i.e. the final infiltration rate of the subsoil. This simplification effectively accounted for preferential infiltration during surface irrigation. Furthermore, this model represented only the dominant processes contributing to deep percolation and therefore required significantly less input data than a Richards' equation model.

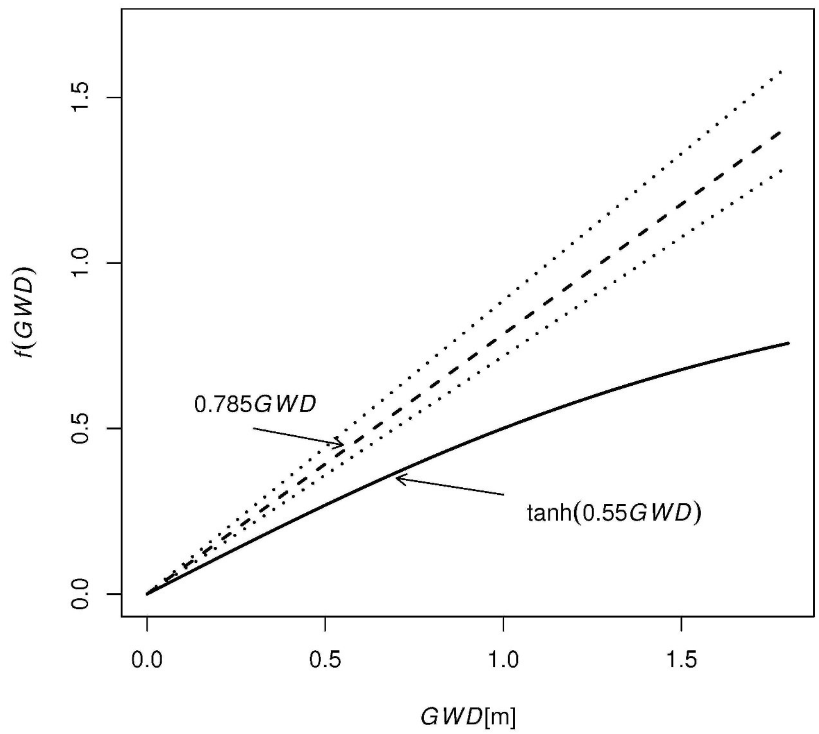

Figure 7: *Factor representing watertable influence f(GWD) for Genetic Programming model $DP = i_f\ t_o\ a\ GWD$ and for our model (equation (2), with $GWD_0 = 1$ m). Dotted lines represent the bootstrap 95% confidence interval for the empirical coefficient of the Genetic Programming model.*

Genetic Programming was applied to analyse data from lysimeter experiment and to test the structure of our model of deep percolation. Genetic Programming finds functional relationships between system inputs and response (deep percolation) directly from observations. In principle, Genetic Programming works with a number of solution sets, rather than a single solution at any one time. It used the operations of mutation and crossover to continuously refine the set of solution, i.e. the functional relationship between deep percolation and its potential drivers.

Using Genetic Programming, a simple model of deep percolation $DP = i_f\ t_o\ a\ GWD$ with model coefficient $a = 0.785$ was recurrently evolved in multiple Genetic Programming runs. It was the best fitting model that was still interpretable in physically meaningful terms. The Genetic Programming model supported the model structure of our formulation given by equations (1) and (2). Particularly, it confirmed our inference on the dominant process contributing to deep percolation, i.e. steady-state percolation during irrigation. Note that the factor representing the watertable influence was slightly different (Figure 7). For the Genetic Programming model, this watertable factor was consistently larger than for our model, with increasing differences for deeper watertables. These differences occurred because, in contrast to our model, the Genetic Programming model did not represent nonsteady-state percolation during redistribution. This lack of representation was obviously compensated by a larger watertable influence on deep percolation.

2.4. Regionalisation of parameters for the model of deep percolation

The following section presents selected results from the journal paper by *Selle, Wang and Mehta* [2011]. For additional or more detailed information please see the appendix F.

The final infiltration rate of the restricting subsoil was the main driver of deep percolation in the lysimeter experiment as it governed steady-state percolation during surface irrigation, which was dominating for most soils [*Bethune, Selle and Wang*, 2008]. For a regionalization of this model parameter and soil hydraulic properties, a study was carried out in the Shepparton irrigation region. A total of 34 soil types were selected and soil hydraulic and basic soil properties were measured at 79 sites. These represented 75% of the total area of the Shepparton irrigation region. More specifically, a total of 250 local scale measurements of final infiltration rates of the subsoil and its basic soil properties were taken. A ring infiltrometer of 350 mm diameter was used to measure final infiltration rates.

Locally measured final infiltration rates displayed poor correlation with all collected basic soil properties (Figure 8). It therefore appeared infeasible to regionalize final infiltration rates for the Shepparton irrigation region using data on basic, physical and chemical soil properties that is often readily available from soil maps. In contrast to final infiltration rates, the other soil parameter of our model, i.e. soil water stored in the rootzone between saturation and field capacity, could be regionalized with a reasonable accuracy. Unfortunately, it was of minor importance for the estimation of deep percolation as most recharge happened, at least in the lysimeter experiment, during irrigation events when percolation processes were not driven by soil retention properties.

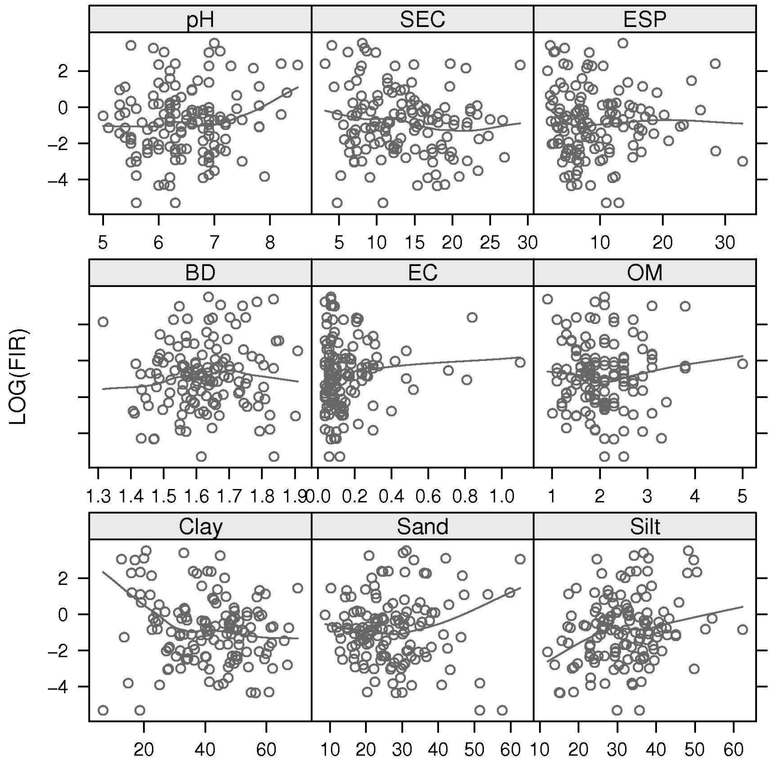

Figure 8: *Scatterplots of ln-transformed final infiltration rates of the various measured subsoils against its basic soil properties: BD is bulk density, Clay is clay content, Silt is silt content, Sand is sand content, OM is organic-matter content, EC is electrical conductivity, SEC is sum of exchangeable cations and ESP is exchangeable-sodium percentage.*

2.5. Concluding remarks

We formulated and tested a model of deep percolation under surface irrigation, which effectively represented dominant processes with a minimum number of model parameters and inputs. However, to estimate deep percolation at larger scales such as for the entire Shepparton irrigation region, these modelling approaches have the following three shortcomings.

Firstly, our effective model was still inferred from lysimeter data. In that way, it may provide limited information on regional scale deep percolation because upscaling of point data to field and regional scale processes is required. We could assume that processes for an irrigated field are the same as observed in the lysimeter experiment. However, the reliability of this assumption will remain unknown.

Secondly, the models presented in this chapter are inappropriate for irrigated landscapes under change with perhaps more heterogeneous landuse and management. This is because these methods were mainly designed for estimating recharge for continuously irrigated landscapes with relatively uniform land use (predominantly perennial pasture) and shallow watertable conditions.

Finally, regionalisation was difficult for the most important model parameter, i.e. the final infiltration rate of the subsoil. However, we also demonstrated why field-scale estimates of final infiltration rates, obtained by fitting a model for surface irrigation to field measurements, may be better correlated with basic soil properties [*Selle, Wang and Mehta*, 2011]. I propose this as a way forward to tackle the regionalisation problem.

Overall, I believe that these studies of deep percolation in the Shepparton irrigation region, although being innovative, highlighted specific challenges of bottom-up modelling strategies. The innovation of this series of studies is perceived to lie in the demonstration of how much one could simplify the system under study focusing only on the dominant processes and key variables. This cascade of simplifications led to a model that provided interesting insight into our experimental and field data sets. However, the application of the model to quantify deep percolation in the Shepparton irrigation region will have particular limitations. Over-simplification is a potential issue for bottom-up modelling.

3. Combining bottom-up and top-down modelling approaches

3.1. Salt mobilisation from the Barr Creek catchment, south-eastern Australia

3.1.1. Background and motivation

Enhanced recharge under irrigated agriculture in the southern Murray-Darling Basin of Australia over the past 100 years contributed to shallow watertables of less than 2 m below the ground surface [*Chiew and McMahon*, 1991]. Shallow watertables play a major role in salinisation of the Murray River as they promote groundwater discharge into watercourses or drains intercepting shallow groundwater [*Duncan et al.*, 2008].

The irrigated Barr Creek catchment in the southern Murray-Darling Basin of Australia was studied to understand groundwater discharge into deeply incised drains, the process dominating salt mobilisation from the catchment. The study catchment has an area of 600 km^2 of which, in a typical irrigation season, more than one half is irrigated. It is characterized by an extremely flat topography. The catchment typically features a 1–2 m deep watertable which intersects a surface drainage network with major drains as deep as 2.5 m. The main catchment drain is Barr Creek. The climate is semi-arid, with hot summers. The average annual amount of irrigation water applied to the study catchment (340 mm) is similar to the amount of average annual rainfall, which however mainly falls in winter whereas irrigation is mainly applied in summer. The dominant land cover has traditionally been perennial pasture. Pasture is usually surface irrigated. Light sandy soils are typically more intensively irrigated and more productive than finer textured soils, mainly due to increasing soil salinity with finer textured soils. The hydrogeology of the study catchment comprises two major units, the Shepparton Formation and the underlying Deep Lead aquifer. The Shepparton Formation forms a complex and heterogeneous aquifer-aquitard system on top of the semi-confined Deep Lead aquifer, which is the major aquifer of the region and mainly consists of gravel and sand. The volume of groundwater discharging into the deeply incised drains is relatively small (10 mm/year on average) compared with the total flow (70 mm/year on average); however, due to the extremely high groundwater salinity (similar to seawater), the amount of salt mobilised through groundwater discharge is substantial.

3.1.2. Top-down modelling approach

The following section presents selected results from the papers by *Selle, Thayalakumaran and Morris* [2010] and *Selle and Hannah* [2010]. For additional or more detailed information see the appendices B and C.

At the beginning of our study of the Barr Creek catchment, we asked a question that is probably typical for top-down approaches: Which variables, related to catchment hydrology, have a detectable correlation with the observed, monthly salt loads at the catchment outlet, and hence might be useful in a model describing salt loads? We found, using a CART analysis of a comprehensive, catchment scale data set, that rainfall, potential evapotranspiration and hydraulic heads of deep regional aquifer were associated with the observed salt loads. Salt loads lagged behind their potential drivers by one month. Surprisingly, no link was detected between salt loads and the irrigation water use in the catchment. Already from a visual inspection of the catchment time series (Figure 9), dynamics of salt loads appeared to be related to rainfall whereas a declining magnitude of salt loads from the mid 1990s seemed to be associated with the decreasing hydraulic head in the deep regional aquifer system.

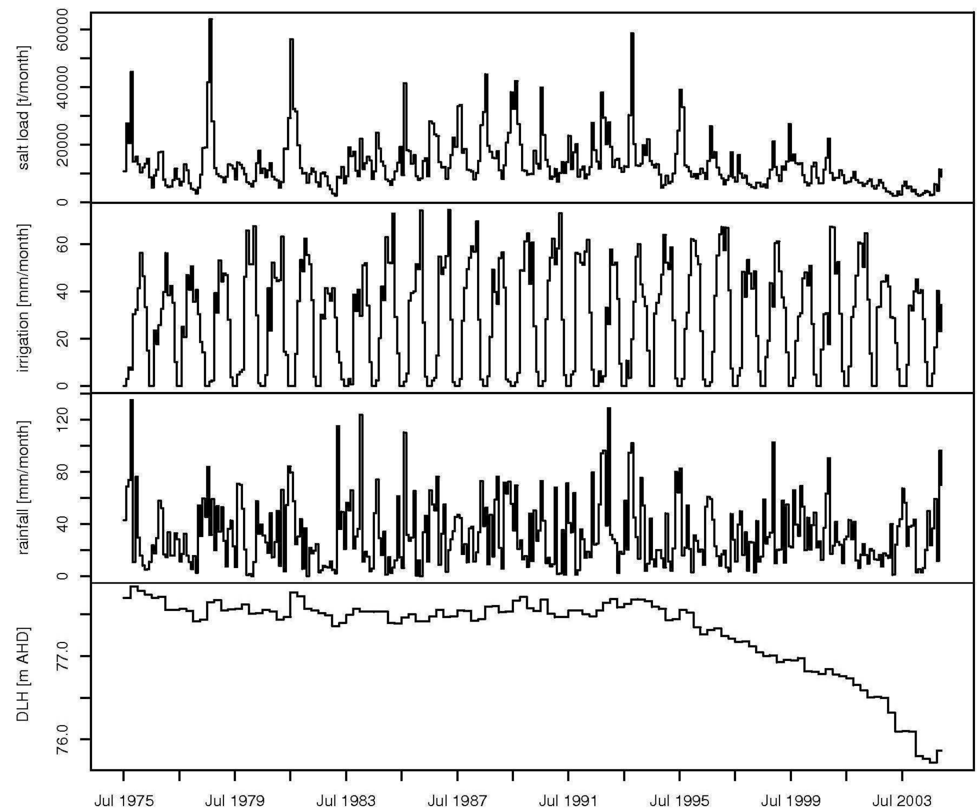

Figure 9: *Selected monthly time series for the Barr Creek catchment. DLH is the hydraulic head in the Deep Lead aquifer.*

Using the key variables indentified from the CART analysis, a conceptual model of salt loads was formulated. In brief, we conceptualised that most of the rainfall water would be transpired by vegetation or evaporated from the soil surface, some rainfall would recharge the groundwater system and subsequently discharge into the deep drains. Some rainfall could also percolate through to the deep aquifer if the hydraulic conditions were favourable. The conceptual model is given by:

$$Q_t = P_t\left(aDLH_t + bPET_t + c\right), \text{ subject to: } 1 \geq \left(aDLH_t + bPET_t + c\right) \geq 0\,, \qquad (3)$$

$$S_t = \left[1 - \exp(-1/\tau)\right]\, Q_t + \exp(-1/\tau)\; S_{t-1}\,, \qquad (4)$$

where Q_t is monthly rainfall recharge to the aquifer system which subsequently becomes discharge (hereinafter referred to as “rainfall recharge”), P_t is monthly rainfall, DLH_t is hydraulic head in the Deep Lead aquifer at month t, PET_t is monthly potential evapotranspiration, a, b, c are empirical coefficients determining the rainfall recharge, S_t and S_{t-1} are discharge rates at month t and $t-1$ respectively, and τ is a time constant. For simplicity, it was conceptualised that rainfall recharge decreases linearly as DLH decreases and/or PET increases. To compute the salt load at the catchment outlet, groundwater discharge S obtained from equations (3) and (4) was multiplied by the average groundwater salinity measured in the catchment. Note that equation (4) can be understood as a is a discrete-time representation of a linear reservoir with an inflow Q, an outflow S and a time constant τ, which can be defined as the time taken for the peak in outflow of a linear reservoir to recess to exp(-1) of that peak value.

When we fitted and cross-validated the conceptual model of salt loads, we observed reasonable model simulations with no significant pattern left in the model residuals (Figure 10).

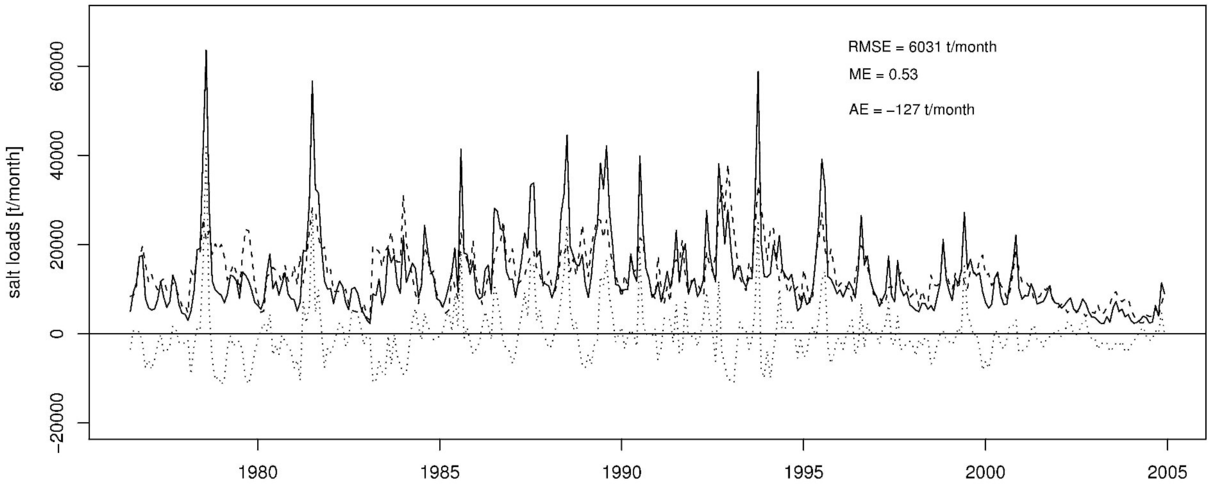

Figure 10: *Conceptual modelling of salt loads at the catchment outlet. Solid line is observed salt load, dashed line is predicted salt load and dotted line is model residuals. Performance of the conceptual model was assessed using the Nash-Sutcliffe model efficiency (ME), the root-mean-square error (RMSE) and the average error (AE).*

Reasonable parameter estimates were obtained for model parameters a, b and c. This was observed from plausible magnitudes of the proportion of rainfall contributing to Q between 0.5 and 3.5 %, and the positive and negative values of a and b, respectively, which represented the conceptualized impacts of DLH and PET on Q (Figure 11).

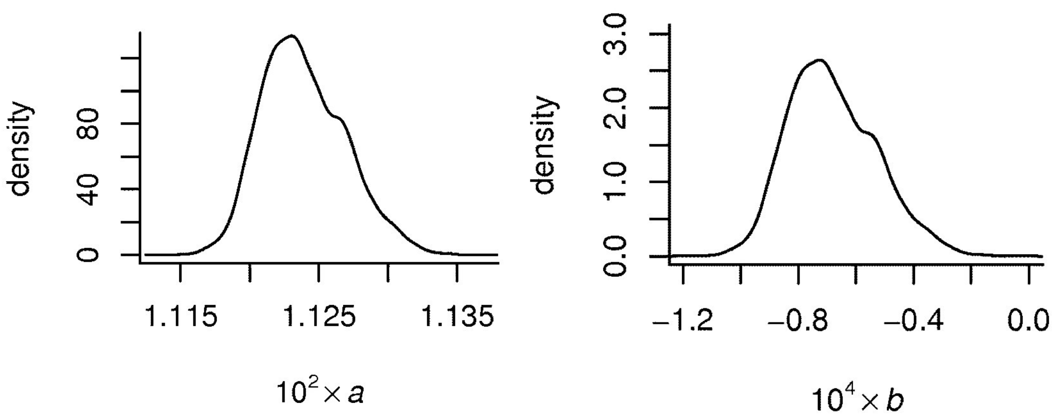

Figure 11: *Kernel density plots of each 5,000 bootstrap estimates for parameters a and b.*

From the conceptual model and its parameter estimates we inferred that, from 1975 to 2004, it was rainfall rather than irrigation that governed salt mobilisation from the Barr Creek catchment. From the mid 1990s to mid 2000s, decreasing Deep Lead heads reduced salt loads exported from the Barr Creek catchment. Note that these two statements were based on a pure top-down view.

3.1.3. Bottom-up modelling approach

The following section presents selected results from the paper by *Githui, Selle and Thayalakumaran* [2012]. For additional or more detailed information see the appendix G.

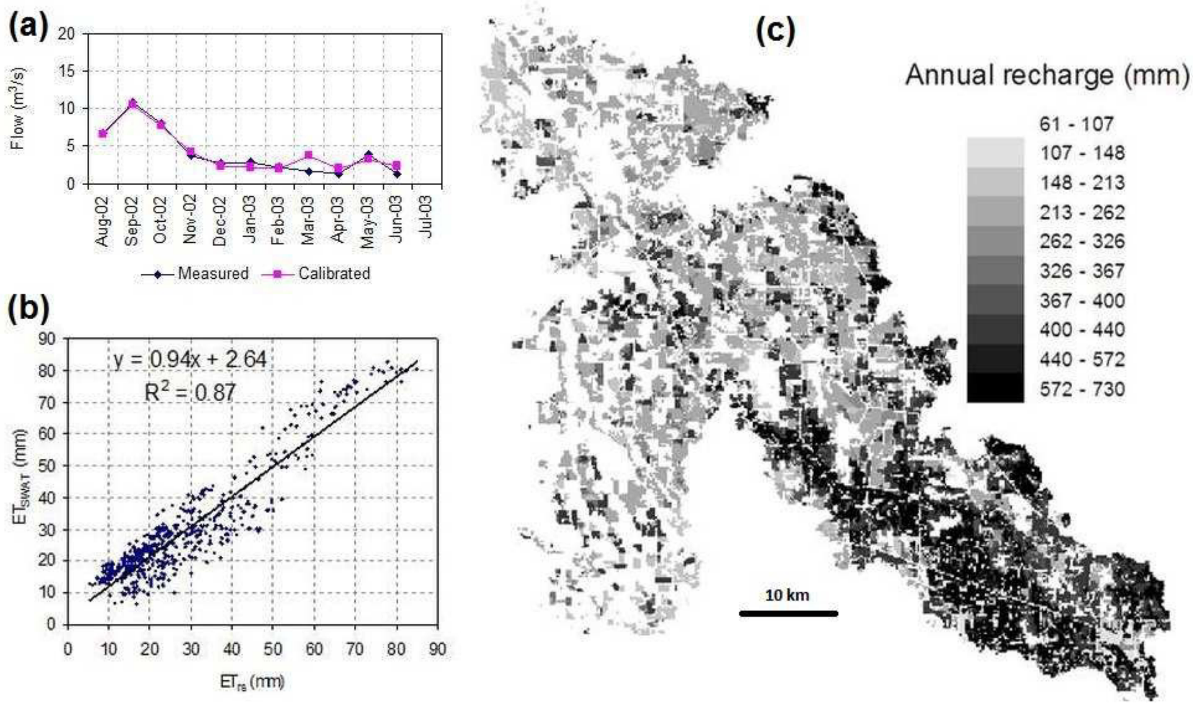

Figure 12: *Calibration results of the SWAT model in 2002/03 (a) for monthly flow in Barr Creek at the catchment outlet and (b) monthly data of remotely sensed evapotranspiration at subcatchment scales; (c) annual recharge estimates from SWAT for the calibration period.*

The Soil and Water Assessment Tool (SWAT), a well tested and widely used spatially explicit hydrological model, was used to quantify groundwater recharge for different landuses and soils of the Barr Creek catchment under the relatively dry climatic conditions of 2002 to 2004. The focus was on groundwater recharge as it drives groundwater discharge processes which in turn govern salt loads exported from the Barr Creek catchment. As required for the implementation of SWAT, the catchment was first split into multiple subcatchments according to the terrain and drain network. Each subcatchment was then further split into multiple hydrological response units (HRUs) based on soil and landuse in each of the subcatchments. Precisely defined, an HRU is a nearly uniform patch of land with a unique combination of soil and landuse. It is the basic modelling unit in SWAT. Additional model inputs were spatially distributed climatic data and irrigation water use. SWAT accounts for a large number of plant, soil, groundwater and stream processes. We ran SWAT at a daily time step. Model parameters were estimated through calibration against a comprehensive set of available data, i.e. monthly flow in Barr Creek and monthly estimates of remotely sensed evapotranspiration aggregated at subcatchment scales. The model-independent parameter estimation and uncertainty analysis tool PEST was used for model calibration.

SWAT was able to simulate observed monthly drain flow and spatially distributed, remotely sensed evapotranspiration (Figure 12). Recharge estimated using SWAT tended to be higher for irrigated landuses, such as perennial pasture, than for non-irrigated land. Recharge for the dry 2002/2003 season was substantial and also higher than what was previously estimated under wetter climatic conditions using the top-down modelling approach. The optimized soil parameters indirectly reflected water flow bypassing the soil matrix that could be responsible for this substantial amount of recharge. Therefore changes in soil characteristics, i.e. the formation of cracks, were likely responsible for the increase in recharge under dry conditions.

3.1.4. Synthesis of top-down and bottom-up modelling approaches

Both the top-down and bottom-up modelling approaches gave different but complementary insights into groundwater recharge and discharge and hence salt mobilisation processes for the Barr Creek catchment. A synthesis of these results was possible because they had some overlap in time. Under relatively wet conditions from the mid 1970s to the mid 1990s, which were the focus of the top-down analysis, rainfall likely governed groundwater recharge and salt mobilisation. There may have been a limited impact of irrigation on salt export. For below average rainfall conditions from the mid 1990s to the mid 2000s, which were focus of the bottom-up modelling, recharge from irrigation increased but leakage of groundwater to the Deep aquifer caused salt loads to decline. The latter point was contributed by the top-down analysis. Plausible causes of declining hydraulic heads in the deep aquifer include intensive pumping in the southern Murray-Darling Basin, closer to the recharge area of the Deep Lead aquifer [*Goode and Barnett*, 2008]. Overall, the first case study demonstrated that only a synthesis of top-down and bottom-up modelling approaches provided a more complete picture of the relevant processes governing salt mobilisation from the Barr Creek catchment.

3.2. Groundwater processes in the Ammer catchment, south-western Germany

3.2.1. Background and motivation

The Ammer catchment in south-western Germany is extensively used for drinking-water production from a karstified carbonate aquifer. The Ammer River is a northern tributary of the Neckar River with an average discharge of 1 m^3/s, which is mainly of groundwater origin. Figure 13 shows the catchment (180 km^2) contributing groundwater to the Ammer River at Pfäffingen gauging station, which is also a groundwater protection area. 70% of the catchment is used for agriculture and 17% are urban areas. The hydrogeology of the Ammer catchment features two main aquifers, the Upper Muschelkalk and the Gipskeuper, both of them up to 100 m thick. The Upper Muschelkalk is a limestone aquifer and the Gipskeuper is characterised by gypsum layers. Both of the aquifers are partly karstified; and the limestone aquifer is the one used for drinking-water production from a total of four production well sites (W1-4, Figure 13). In this study, we aimed at an understanding of processes governing selected aspects of groundwater quality in the Upper Muschelkalk aquifer of the Ammer catchment.

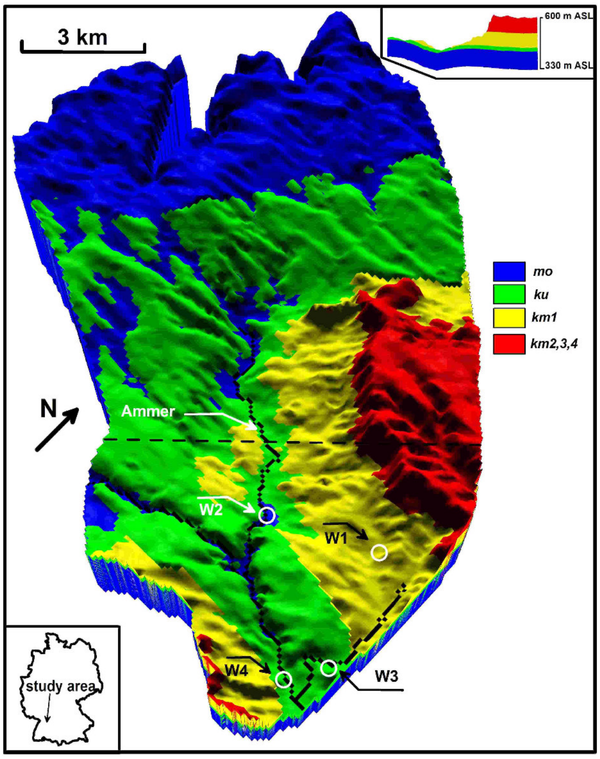

Figure 13: *Ammer catchment with drinking-water production well sites (W1-4), the Gipskeuper (km1), the Lettenkeuper (ku) and Upper Muschelkalk (mo) aquifers. Schönbuch Plateau is the area displayed in red (km2,3,4). Inset in the upper right corner shows a cross-section; and the dashed line indicates its approximate location.*

3.2.2. Top-down modelling approach

The following section presents selected results from the papers by *Selle, Schwientek and Lischeid* [2013] and *Pavlovskiy and Selle* [submitted]. For additional or more detailed information see the appendices I and J.

The starting point for our top-down analysis was water quality data collected from seven wells representing groundwater from the Upper Muschelkalk aquifer in the Ammer catchment. Note that these seven wells also included the drinking-water production wells. We analysed data of major ion chemistry, redox-sensitive variables and environmental tracers indicating groundwater age. Environmental tracers are typically applied to catchments by natural precipitation with a known input time series and transport behaviour, which allows the estimation of transit times of water. We also investigated organic mircopollutants, but they were not detected in the wells. Groundwater quality data from the Ammer catchment were analysed using principal component analysis (PCA). For PCA, normalised observations (deviations from the mean) are expressed as linear combinations of uncorrelated principal components. Principal components were often found to be interpretable as processes governing observations. This can be explained using an example: if nitrate and pesticides concentrations are observed to correlate for a number of groundwater wells, there is probably a common process that is causing these variables to link; and this process (which may be leaching from agricultural soils in this particular case) will then be represented by a principal component. Mathematically, normalised observations are expressed as the product of the matrix of principal component scores and the transpose of the matrix of loadings, which represent coefficients of correlation between principal components and the original water quality variables. Note that there are no real processes assumptions involved in a PCA, but one often gains information on the occurrence and the importance of processes from this type of analysis.

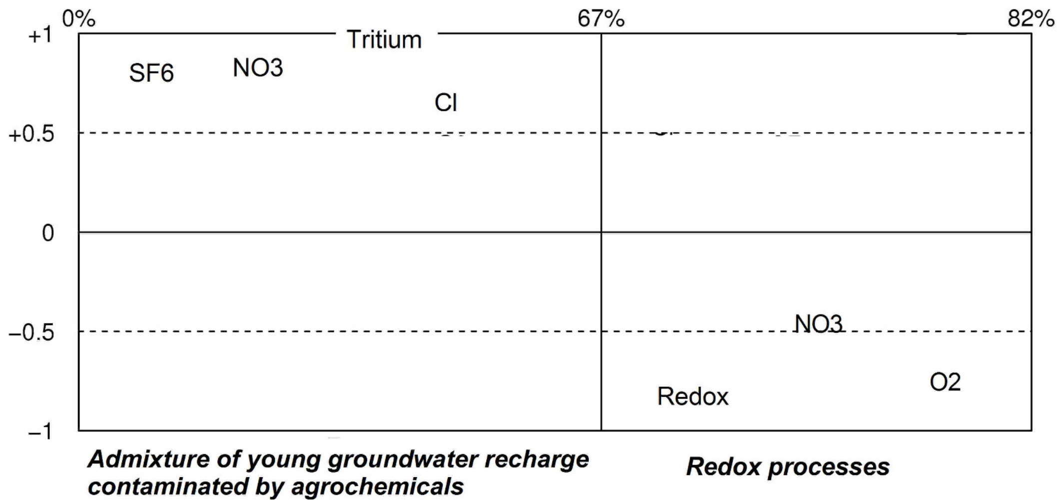

Figure 14: *Loadings from PCA of water quality data from Upper Muschelkalk wells. Explained variances for the two most important principal components are displayed horizontally and the loadings vertically. SF6: sulfur hexafluoride, NO3: nitrate, Tritium: tritium, Cl: chloride, Redox: redoxpotential and O2: dissolved oxygen.*

Figure 14 displays results of PCA of water quality data from the Upper Muschelkalk wells, and more specifically, computed loadings are presented.

The first principal component displayed high positive correlation with environmental tracer concentrations (tritium and sulfur hexafluoride) and also with nitrate and chloride concentrations. The latter indicates an influence of agrochemicals. We therefore interpreted this component as relatively young groundwater recharge polluted by agrochemicals. This component is probably admixed to an older, clean groundwater component representing the average water quality in the wells. As mentioned before, for PCA, we interpreted deviations from the mean; and the average water quality in the wells is likely represented by an old, clean water component. A second principal component was highly correlated with redox-sensitive variables. We interpreted this principal component as redox processes driven by microbial activity.

It is interesting to note that both of the computed principal components influenced nitrate concentrations (Figure 14). The principal component interpreted as an admixture of young groundwater contaminated by agrochemicals was obviously more important for explaining the observed deviations from the mean nitrate concentrations than the principal component interpreted as redox-processes. This can be seen from a higher correlation of nitrate with the first than with the second principal component.

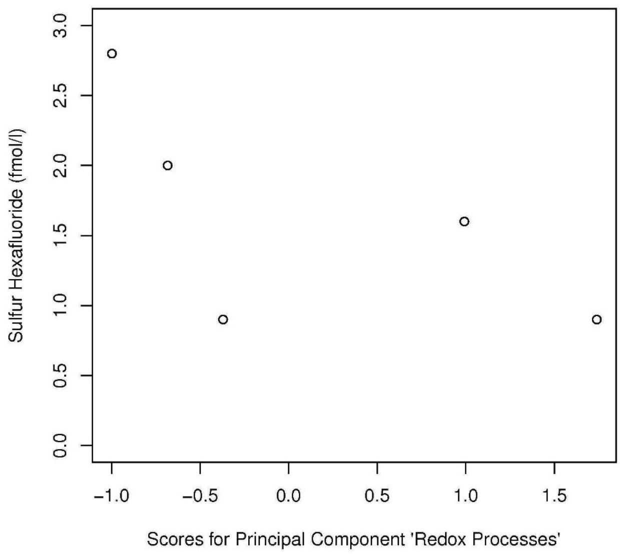

Figure 15: *Plot of scores for principal component interpreted as 'redox processes' versus independently measured sulfur hexafluoride concentrations, i.e. they were not used in the original PCA.*

If principal components are interpretable as processes then scores can be understood as process magnitudes. In Figure 15, the scores for the principal component interpreted as redox processes are shown. We observed a lack of significant correlation between the sulfur hexafluoride concentrations, as a proxy of the transit time of groundwater to the wells, and the scores for the principal component interpreted as redox processes. This indicates that these processes equally affected both young and old groundwater components. In summary of the PCA, we found that groundwater quality in the Upper Muschelkalk wells was governed by mixing of a polluted and relatively young and a substantially older and relatively clean water component. Both of these groundwater components were probably equally affected by redox processes, which likely lead to attenuation for some of the pollutants.

As a second step of the top-down analysis, we further characterised the young and old groundwater components identified from PCA. More specifically, we attempted to localise those water components contributing groundwater to the drinking-water productions wells. There were three findings from this analysis that turned out to be relevant here.

Firstly, we noted that water from all production wells had substantially lower sulfate concentrations compared to water from the Gipskeuper springs. This indicates that Gipskeuper overburden plays a minor role in the recharge source areas of the production wells. In Figure 13, the area not covered by Gipskeuper is displayed in green and blue colours. This area is the potential recharge source area for the drinking-water production wells.

Secondly, we examined additional data for two selected production well sites. The Breitenholz site (W1, Figure 13) had an elevated groundwater temperature and relatively low tracer concentrations for both tritium and sulfur hexafluoride. This suggested a long, >50 years and deep groundwater flow paths with insignificant recharge on the way from its recharge area to the well. This can only be the area north of the Schönbuch plateau (Figure 13). On the other hand, the Poltringen site (W4, Figure 13) had a continuous transit time distribution with short and also long transit times, and a mean transit time of 10 years. This indicated a different recharge source area than for Breitenholz site, which is likely the remaining blue and green area in Figure 13, i.e. the area west of the Ammer River and the Reusten anticline.

Finally, we found that water in the other production well sites, other than the two sites discussed previously, can be represented as a mixture of two types of water. These types of water were the old water from the Breitenholz type and the young water from the Poltringen type.

Piecing all three findings together (Figure 16), there were two main sources of groundwater to the wells: relatively clean groundwater, mostly recharged > 50 years ago from north of the Schönbuch, and a relatively young groundwater component with a mean transit time of 10 years coming from west of the Ammer River and the Reusten anticline. The young groundwater component is contaminated by agrochemicals and mixes with the old groundwater at each well site with different proportions.

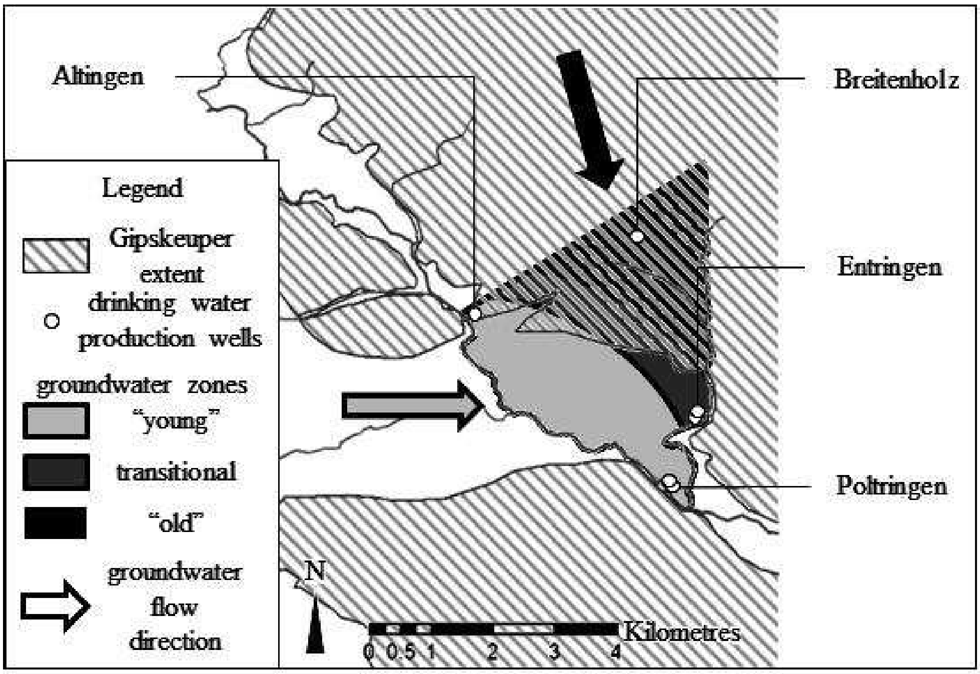

Figure 16: *Conceptual model of groundwater flow to drinking-water production well sites in the Ammer catchment.*

3.2.3. Bottom-up modelling approach

The following section presents selected results from the paper by *Selle, Rink and Kolditz* [2013]. For additional or more detailed information see the appendix H.

The conceptual model of groundwater flow from the top-down analysis (Figure 16) provided only a coarse picture of groundwater flow that could be significantly refined using a bottom-up modelling approach. Here we applied a 3-dimensional, steady-state groundwater model. The groundwater model was set up as an OpenGeoSys model in collaboration with Helmholtz Centre for Environmental Research UFZ. This model included a detailed structure of the subsurface and a set of appropriate boundary conditions. Hydraulic conductivities for the different hydrogeological units were calibrated using observed groundwater heads in the various units.

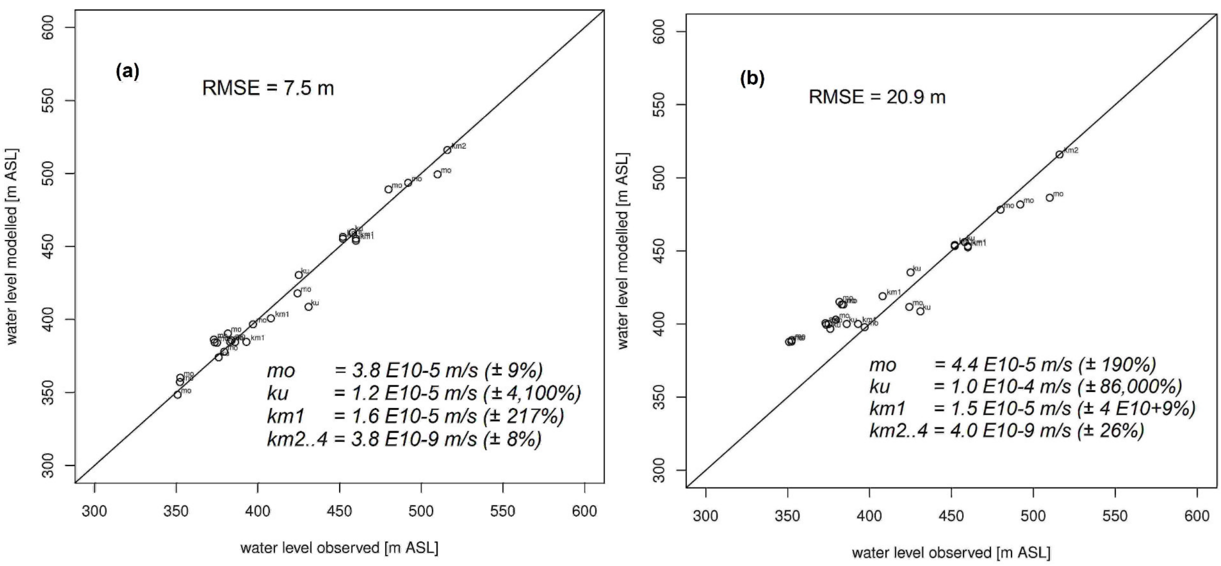

Figure 17: *Observed versus fitted groundwater levels for two scenarios: (a) groundwater discharge as a diffuse process via the entire River bed and (b) via discrete points at springs. Hydraulic conductivities calibrated for the various units (see Figure 13 for notation of units) are also displayed. Performance of each scenario was assessed using the root-mean-square error (RMSE).*

For groundwater modelling in the Ammer catchment, we represented two plausible discharge scenarios to test hypotheses on groundwater flow. More specifically, we tested (i) a discharge scenario that conceptualised groundwater discharge as a diffuse process via the river beds of the entire stream network and (ii) another discharge scenario representing discharge via discrete points at springs. These scenarios were calibrated against observed water levels. A plot of observed versus simulated water levels can be seen in Figure 17. Different fits were obtained for the two discharge scenarios. Fit for the discharge via springs was substantially worse than for discharge via the entire beds of Rivers and Creeks.

A completely different perspective on the two scenarios is obtained if flow paths and transit times of groundwater, computed using particle tracking, were examined (Figure 18). The discharge scenario that did not really fit water levels (“spring discharge scenario”), resulted in flow paths of groundwater that matched the conceptual model of groundwater flow from the top-down approach. Young groundwater coming from west of the Ammer River, displayed in light grey, and old groundwater from north of the Schönbuch, displayed in dark grey, are observable (Figure 18b). For the "spring discharge scenario", the misfit to water levels is probably tolerable (Figure 17b), because a steady-state groundwater model was applied but water levels were observed at different times. Furthermore, locally measured water levels have a limited meaning for these heterogeneous, partly karstified aquifers.

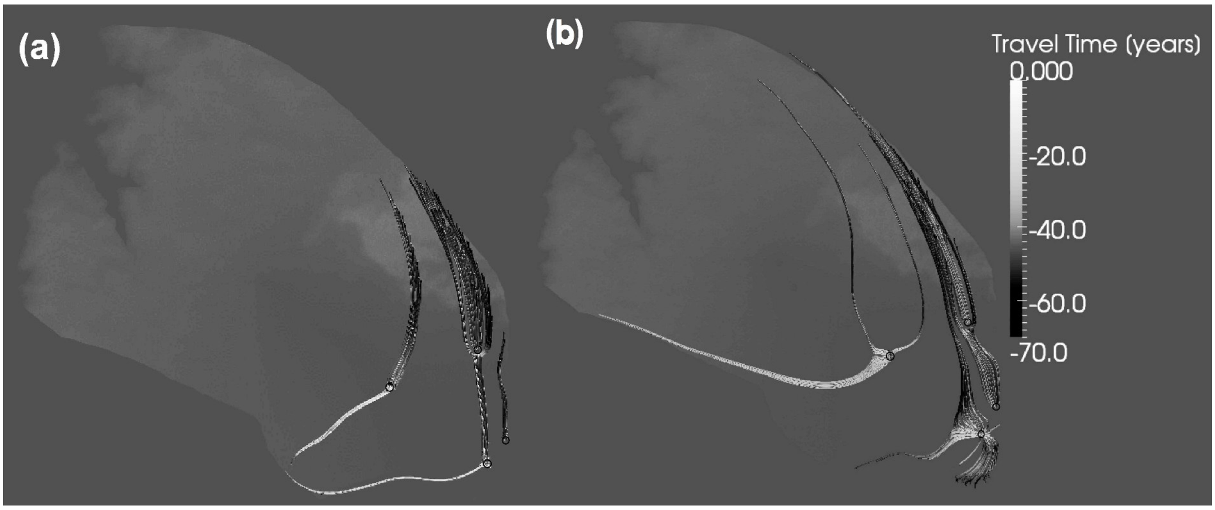

Figure 18: *Horizontal plane projection of flow paths and travel times to drinking water production wells, computed using particle tracking methods, for the same two scenarios, (a) and (b), as displayed in Figure 18. One can see the outline of the Ammer catchment. Wells are displayed as black circles; flow paths and transit times are displayed in different shades of grey.*

3.2.4. Synthesis of top-down and bottom-up modelling approaches

From a synthesis, we obtained a relatively reliable understanding of the processes dominating the investigated aspects of water quality for the Upper Muschelkalk aquifer, particularly for the drinking-water production sites. There are two main sources of water to the well sites: relatively clean groundwater, mostly recharged > 50 years ago, from north of the Schönbuch and a relatively young groundwater contaminated by agrochemicals from west of the Ammer River. Old and young groundwater components are subject to attenuation processes. Groundwater quality at the wells is still good because of the significant proportion of old groundwater and some attenuation of pollutants. However, water quality may deteriorate in the future.

Top-down and bottom-up modelling approaches were again complementary for this second case study. Looking at the fits of the groundwater flow models to observed water levels exclusively, would have resulted in a misleading perception of groundwater flow. The conceptual model from top-down type of analysis was highly beneficial for a model selection. Using the bottom-up approach, we obtained a more detailed picture of flow paths and transit times than from the top-down approach.

3.3. Concluding remarks

A major problem of top-down modelling approaches is that these apply mostly statistical methods analysing and explaining variability rather than the observed mean values. For a case when the data set being analysed has little explainable variability around the mean values, one would be unable to detect and quantify processes with a very constant magnitude if they were linked to those mean observed values. An example from the first case study would be a “constant dripping” of recharge from irrigation and a resulting base level of salt load that would be invisible for the CART analysis. On the other hand, these hardly varying processes can be readily quantified, e.g., from a water balance; and bottom-up type of approaches are typically based on these kind of universal balance laws. A similar example highlighting potential limitations of top-down approaches was presented in the second case study, where a PCA was used to explain observed deviations from mean water quality variables. The average water quality in the wells was probably best represented by its main water source. This water source remained undetected by PCA. However, the contribution from this water source could be quantified using a groundwater flow model.

Based on my experience, I cannot always recommend using observations straight away for calibration of complex, bottom-up type of models. A model selection based on the goodness of fit to the raw data can be misleading. This was demonstrated for the second case study, where a groundwater flow model was calibrated to observed water levels. A useful, alternative approach is to apply top-down approaches as a pre-processing of the available data set and then to use the resulting conceptual model to test spatially explicit catchment models. A model selection based on this pre-processed information could be better. The outcome of a top-down analysis is typically more insightful in terms of the underlying system processes than just the raw data. This pre-processing of data will likely result in a better model selection than a model choice based on a fit to data with an unknown uncertainty. In contrast to deterministic, bottom-up type of modelling, the data uncertainty is naturally accounted for in statistical techniques as they are often applied for top-down approaches.

From a purely technical point of view, the syntheses presented in this chapter can also be understood as a combination of statistical and deterministic modelling approaches. In principle, these techniques can be combined in three possible ways: (i) to use statistical methods as a pre-processing tool for deterministic modelling as we did in the case studies presented in this chapter, (ii) as a statistical post-processing of the results coming out of deterministic modelling and (iii) as a direct integration of the statistical methods into deterministic modelling approaches. Examples of (ii) relevant to hydrology include, e.g., weather forecasting with ensemble methods [*Gneiting and Raftery*, 2005]. An example of (iii) is the study by *Liao and Cirpka* [2011], who modelled solute transport in the streams undergoing hyporheic exchange. Transport of solutes in the river was represented by a deterministic advection-dispersion equation whereas travel times through the hyporheic zone were described as statistical distributions.

Using two catchment studies, I demonstrated that it is possible to obtain an understanding of flow and transport processes at catchment scales - that is both detailed and reliable – from a combination of top-down and bottom-up approaches. Relying on only one of the two approaches would likely result in a misleading or incomplete picture of the relevant hydrological processes. Looking on the same system from different angles is not a waste of time but can be highly useful; and our analysis in both the Ammer and the Barr Creek catchments provided useful information for water management. I therefore believe that the dominant hydrological processes in catchments, the understanding of which is required for a proper management of fresh water resources, may be discovered by a synthesis of top-down and bottom-up approaches.

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