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# The influence of conceptual geological models on the simulation of flow and transport in Quaternary aquifer systems

Ph.D. thesis 2004

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# Preface

The present thesis has been submitted as a part of the Ph.D. degree at the Technical University of Denmark. The thesis includes an introduction, three brief summaries, conclusions and perspectives and three manuscripts that constitute the actual scientific work.

The study has taken place at the Department of Hydrology, Geological Survey of Denmark and Greenland (GEUS) in cooperation with Environment & Resources (DTU). My supervisors are Professor Karsten Høgh Jensen and Associate Professor Peter Engesgaard both at Geological Institute (University of Copenhagen), Professor Jens Christian Refsgaard, Department of Hydrology (GEUS) and Flemming Larsen at Environment & Resources (DTU). I gratefully acknowledge my supervisors for their inspiration, competent guidance and never failing support. As a part of the study, six months were spent at the Land, Air & Water Resources (LAWR) (University of California, Davis) with Graham E. Fogg as my formal supervisor. The work at Dalum well field (manuscript one) would not have been possible without assistance from Odense Vandselskab a/s, Bjarne Madsen (WaterVision) and Kipp Solomon and Alan Rigby (both at University of Utah). I would like, formally and informally, to thank all involved persons at the LAWR, E&R and GEUS and especially my colleagues at Department of Hydrology.

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Copenhagen, November 2004

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The manuscripts are not included in this www-version of the thesis. The complete thesis can be obtained from the Library at the Institute of Environment & Resources, Bygningstorvet, Building 115, Technical University of Denmark, DK-2800 Kgs. Lyngby (library@er.dtu.dk) or directly from the author at the Geological Survey of Denmark and Greenland, Øster Voldgade10, DK-1350 Copenhagen K (ltr@geus.dk).

# Abstract

This dissertation investigates several issues related to conceptualization of complex aquifer systems and its effect on groundwater transport predictions. The thesis focuses on regional scale multi-aquifer systems of Quaternary deposit, typically for aquifer systems in the eastern part of Denmark.

In the first manuscript “Simulation of age and environmental tracer concentrations in a complex shallow aquifer”, the use of environmental tracers as a constraint in groundwater models is evaluated. The study investigates to what extent the age method is transferable to complex aquifer systems and develops a methodology that can take advantage of environmental tracer concentration observations directly.

In the second manuscript “The importance of alternative conceptual models for simulation of concentrations in multi aquifer systems”, the influence related to deterministic conceptualizations on prediction uncertainty is examined. Conceptualizing a complex multi-aquifer system involves different types of hydrogeological information, but well data is probably the most important (if available) at least in physically based modeling. There are, however, many possible methods of interpretations and categorizations of well log information into hydrofacies. In the manuscript it is shown how four common ways of conceptualizing can lead to quite different predictive results, and this despite of the common calibration targets and somewhat identical flow results.

The last part of the thesis includes the manuscript “Application of transition probability geostatistics in hydrogeological modeling of a Quaternary aquifer complex”. Following a methodology that recognizes the relative importance of geological structures, well log information and general geological knowledge, a stochastic method is used as an alternative to deterministic methods in describing geological heterogeneity. The applicability of the stochastic method is tested for complex multi-aquifer systems typically for East-Danish conditions. The predictive capabilities are measured in terms of ability to simulate environmental tracers following the methodology developed in the first manuscript and compared with simulations of alternative conceptualizations from manuscript two.

# Resumé

I denne afhandling er forskellige emner omkring konceptualisering af komplekse aquifer systemer undersøgt, samt hvorledes konceptualiseringen påvirker transport. I afhandlingen fokuseres der på multimagasin systemer i Kvartære aflejringer af regional skala, systemer der er typiske for øst-danske magasin forhold. Afhandlingen består at tre manuskripter der hver for sig og i sammenhæng beskriver forskellige problemstillinger relateret til modellering af magasin systemer på regional skala.

I det første manuskript ”Simulation of age and environmental tracer concentrations in a complex shallow aquifer”, undersøges muligheden for at bruge miljø-tracere i model sammenhænge. Der undersøges i hvilken udstrækning anvendelsen af miljø-tracere brugt som aldersdaterings værktøj er gyldig/brugbar når det implementeres i komplekse magasin systemer, og der udvikles en metode der muliggør at bruge miljø-tracer målinger direkte.

I det andet manuskript “The importance of alternative conceptual models for simulation of concentrations in a multi-aquifer system” undersøges usikkerheder relateret til deterministiske konceptualiseringer af geologiske strukturer. Til konceptualisering anvendes flere typer data, hvor den geologiske borings beskrivelse måske er vigtigst, i hvert fald for opstilling af fysisk baserede modeller. Oversættelse af geologiske informationer på punkt niveau til model skala kan ske på et utal af måder. I dette manuskript er det vist hvorledes fire almindelige måder at oversætte borehuls data til model skala, bevirker at der simuleres ret forskelligt hvad angår transport, til trods for at de forskellige modeller er kalibreret til samme datasæt og giver nogenlunde enslydende bud på trykafvigelser.

I det tredje manuskript “Application of transition probability geostatistics in hydrogeological modeling of a Quaternary aquifer complex” undersøges brugen af stokastiske metoder til beskrivelse de Kvartærgeologiske aflejringer. Der anvendes en geostatisik metode der nyttiggør specifik viden og geologiske forhold i direkte sammenhæng med geologiske beskrivelser fra borehul logs. Den stokastiske metode er brugt som et alternativ til den deterministiske metode, og brugt indenfor samme opland. Modellens evne til at simulere bliver sammenholdt med målinger af miljø-tracere under anvendelse af metodikken fra det første manuskript og sammenholdt med simuleringer fra manuskript to.

# Table of content

# Chapter 1 : Presentation of thesis

The thesis is written in article form. Each manuscript is intended for publication or has already been submitted with only minor modifications. The manuscripts can be read individually, however, they all focus on issues related to regional scale hydrological modeling.

- Chapter 2 includes the manuscript “Simulation of age and environmental tracer concentrations in a complex shallow aquifer”.
- Chapter 3 includes the manuscript “The importance of alternative conceptual models for simulation of concentrations in multi aquifer systems”
- Chapter 4 includes the manuscript “Application of transition probability geostatistics in hydrogeological modeling of a Quaternary aquifer complex”

A brief introduction to the subject areas is given in the following. A short summary of the three manuscripts, some general remarks to the findings, and an outlook follow this.

## Introduction and objectives

Integrated hydrological modeling using physically based distributed models is an important tool in management of our water resources, especially with growing focus on sustainability and surface water / groundwater interaction. Physically based hydrological modeling provides the framework for which an increasing amount of data and process understanding can be integrated and compared. In this thesis I investigate issues related to regional scale physically based hydrological modeling. The central questions that are investigated are: How does different geological conceptualizations affect regional sized models, to what extent can we take advantage of subjective information in model context, to which extent are these coherent in at model scale and to what extent do conceptualizations influence the predictive uncertainty.

In hydrological modeling of regional aquifer systems the need for direct and indirect information including geological, hydrogeological and hydrological data is obvious. The model parameterization is accomplished using these data. Especially when dealing with regional scale transport, it is difficult to achieve information. Concentrations of environmental tracers measured in the groundwater can be regarded as an option in this aspect. Present in the groundwater they can be related to heterogeneity of the

flow-field and recharge – much like a large-scale tracer experiment. It is in this aspect that environmental tracers have grown popular among hydrogeologists (Engesgaard and Molson, 1998;Goode, 1996;Portniaguine and Solomon, 1998;Sheets et al., 1998;Varni and Carrera, 1998;Zoellmann et al., 2001). Commonly environmental tracers such as Tritium/Helium-3 ($^3H/^3He$) and chlorofluorocarbons (CFCs) have been translated into apparent age and consequently used in the modeling of a system, see e.g. Busenberg and Plummer (2000) and Cook and Herczeg (1999). Interpretation of environmental tracers into groundwater age relies on the ability to estimated the influence of flow conditions (Maloszewski and Zuber, 1993; Mook, 2000). While this might be straightforward for simple aquifers, it is far more complicated for regional scale aquifers. The applicability of using environmental tracers in complex multi-aquifer systems and to what extent simulation of environmental tracers can be used in assessment of predictive uncertainty are addressed in the first manuscript.

Predictive uncertainty may originate from three main sources: (i) scenario uncertainty (lack of knowledge on future evolution of the system), (ii) model (conceptual) uncertainty, and (iii) parameter uncertainty (Samper et al., 1990). Traditionally, the predictive uncertainty has been expressed as an expansion of parameter uncertainty. Parameter uncertainty is seen as the range at which parameters can be changed without affecting the model ability to match observations (Poeter and Hill, 1998). The complexity of the uncertainty related to conceptualization increases as the model area grows to regional scale.

Beckers and Frind (2000) show, in an investigation of the regional Waterloo moraine complex, that conceptualization is a key issue not only in relation to credibility, but also in relation to usability of simulations. It is recognized that model assumptions, regarding conceptualization of geological features and structures, are of vital importance for simulation of flow and transport at regional scale (Fogg et al., 2000;Martin and Frind, 1998). Neuman and Wierenga (2003) recognized conceptual uncertainty as the dominant source of uncertainty in model predictions. In the second manuscript we investigate to what extent four different geological conceptualizations affect flow, in terms of ability to meet calibration targets of piezometric head and stream discharge, and transport predictions, in terms of simulation of environmental tracer concentrations and more traditional comparison with apparent age observations.

Stochastic models can be viewed as an alternative method of describing geological structures. In de Marsily et al. (1998) a suite of geostatistical simulation techniques to represent geological heterogeneity is said to have immense advantage over traditional

deterministic method. The main reasons being that the geostatistical methods can be fully conditioned to local information and because they limit the level of subjectivity to deal with statistical parameters. For regional scale aquifer systems geostatistical methods that have been applied successfully to aquifers dominated by sand/gravel using TRPOGS (Carle et al., 1998;Fogg et al., 1998;Weissmann et al., 1999;Weissmann and Fogg, 1999). One of the main advantages about TPROGS is that it can employ soft or subjective data directly in estimation of the statistical parameters, which is shown to be of vital importance when dealing with regional scale modeling of aquifer heterogeneity (Carle, 1997;Carle and Fogg, 1996;Carle and Fogg, 1997). In the last manuscript the applicability of the TPROGS on regional scale Quaternary multi-aquifer complex is tested. The predictive capabilities are measured in terms of ability to simulate environmental tracers and the results are compared with simulations of traditional deterministic conceptualizations.

# Thesis summary

## Study areas

The two catchments discussed in this thesis are both of regional extent. The study area of manuscript one is located near Odense on the island of Funen and covers 250 km². The catchment discussed in manuscript two and three covers 600 km² and is located at the southwestern part of Zealand. Both areas are characterized by undulating topography, numerous small streams and their aquifer systems are complex multi-aquifers of glaciofluvial deposit, primary till and sand/gravel. The investigated complexes are typical for the eastern part of Denmark, but the investigated issues are probably of general interest for most Quaternary multi-aquifer complexes.

## Summary of manuscript one

Modeling of groundwater flow and transport requires direct and indirect observations of hydrogeology and hydrology. For transport behavior it is difficult to achieve information especially when dealing with large-scale (regional) models. It is in this aspect that environmental tracers have grown popular among hydrogeologists (Engesgaard and Molson, 1998;Goode, 1996;Portniaguine and Solomon, 1998;Sheets et al., 1998;Varni and Carrera, 1998;Zoellmann et al., 2001). Environmental tracers are present in the nature as a consequence of human activity – Tritium were released with the atmospheric atomic bomb testing in the 1950' and 1960', CFC's as a result of cooling industries, SF6 from high voltage switches and 85Kr from reprocessing of used nuclear fuel rods (Cook et al., 2000;Ferronsky and Polyakov, 1982). Their presence in the precipitation have been monitored since the 1950' at different locations around the world, and the precipitation concentrations of environmental tracers can be reconstructed for most areas on the northern hemisphere, with some degree of uncertainty. Because of this, concentrations measured in groundwater can be related to transport through the system and recharge concentrations –much like a large-scale tracer experiment.

In many cases environmental tracers have been used to date the age of groundwater e.g. the time elapsed from recharge to sampling (Busenberg and Plummer, 1992;Busenberg and Plummer, 2000;Oster et al., 1996;Szabo et al., 1996). The method for determining groundwater ages from environmental tracers involves among other things interpretation that relates measured concentration to recharge period and flow conditions in the aquifer. This interpretative method has proven robust and useful

when applied to homogeneous and shallow groundwater conditions (Portniaguine and Solomon, 1998;Reilly et al., 1994;Szabo et al., 1996). The aim of the manuscript was to investigate the usability of this methodology in a complex aquifer system of regional scale.

Interpretation of environmental tracers into groundwater age relies on assuming that the groundwater ages distribution can be described analytically (Maloszewski and Zuber, 1993;Mook, 2000). The groundwater age distribution is estimated from assumptions regarding flow conditions. In order to investigate the applicability to complex multi-aquifer systems, we developed a methodology for simulating well specific groundwater age distribution using particle tracking. Simulated shape of age distributions depends to some extent on sampling size and whether the system is modeled in transient or steady state, but shape and size were largely driven by the heterogeneity of the model and the topographical variations. For simplicity and transparency sake, diffusion and dispersion was not modeled directly.

The modeling produced age distributions, even for the simple particle tracking without dispersion and diffusion, that were of irregular shape and size without similarity to the assumed age distributions used in the analytical methodologies. Enveloping the modeled age distributions and estimated recharge concentrations it is shown how concentrations of environmental tracers would vary in time at well locations. Assuming that the modeled age distributions are accurate representations of the actual flow and transport of this aquifer complex, it was possible to explore the type of errors associated with the traditional age dating approach. Our analysis shows that derived groundwater ages are dependent on sampling time. This time dependence relates to the non-linearity of recharge concentrations and the shape and size of age distribution that is non-coherent with the simplified assumptions of the traditional approach.

For complex aquifer systems the water follows complicated pathways, causing the age of a given location to consist of a distribution of ages. The interpretation of environmental tracer concentrations to age of groundwater are carried out using simplified assumptions that is not representative for complex flow systems (if any). Constraining of flow models to “age observations” may thus lead to misrepresentations that are biased depending on sampling time. If environmental tracers are used directly in terms of concentrations instead of ages, not only the spatial but also the temporal variations will matter in constraining. Additional measurements at the same location but at different time, would be lost in conversion to age prediction, but can provide additional information if used directly.

## Summary of manuscript two

Conceptualizing aquifer properties is a key component in physically based modeling (Carrera, 1993;Martin and Frind, 1998). Conceptualization is the base characterization that specifies the reference for which model structures and processes should be interpreted and parameterized. For regionally based modeling it is especially aquifer properties and heterogeneity that is the important aspect in conceptualization (Beckers and Frind, 2001;Fogg, 1986). Conceptualizing geological media is somewhat subjective and depends on data availability, modeler experience and indirect data. In this investigation we constructed four different conceptualizations that each is calibrated to flow and discharge data. As a consequence of difference in conceptualization the models have different parameters and residuals as well as different performance in simulation of environmental tracers.

The four models show minor differences in the level of ability to simulate head and discharge observations after calibration. There were no significant differences on spatial residual distributions and the calibrated parameters fall within realistic physical ranges. Differences between models were generally smaller than differences between model and observations, suggesting that other factors not included in conceptualization may influence the flow field. These factors could include difficulties in relating point observations to model scale.

Model capabilities to predict groundwater age and environmental tracer concentrations were compared with 32 observations of environmental tracers. The methodology of constructing age distributions from particle tracking developed in manuscript one is used here. At first environmental tracers were interpreted into age predictors, which were compared to modeled mean ages of the four different models. Then, model predictions of tracer concentrations were compared directly with measurements, following the methodology of manuscript one where recharge concentrations and simulated age distributions are enveloped into concentration predictions.

Comparing environmental tracer ages with simulated ages showed better performance for the simple model of the four. The simple model treated the multi-aquifer system as a single uniform water barring unit, the more complex models had a larger degree of aquifer heterogeneity described. As a consequence the simple model had flow conditions that were in agreement with flow field assumptions used in age predictions from environmental tracers. This is in agreement with the findings of manuscript one; comparing model ages with ages from interpretation of environmental tracers is not straight forward if applied to flow in complex aquifer systems. Direct comparison of

model concentrations and measurements of environmental tracers shows better agreement for the more complex model than for the simple models. The accuracy for any of the models was not impressive for ages and concentrations. Comparing prediction residuals for concentrations with calibration residuals for heads shows that the residuals for the extrapolation step (concentrations) are much larger than the residuals for the calibration step (heads). Differences between the models are of same magnitude as their simulation residuals. The predicted concentration range of the four models encapsulated about half of the observations.

Summarizing the results of manuscript two it may be said: in simulating behavior of observations that are subject to calibration, it may be adequate with a single conceptualization as calibration compensates or hides conceptual errors in the parameter estimation procedure. For predictive purposes when extrapolating from the calibration base, different conceptualizations might produce very different results.

## Summary of manuscript three

Following the investigation of manuscript two the relative importance of conceptualization of geological heterogeneity is recognized as a key element in representing model behavior beyond calibration observations. In manuscript three aquifer heterogeneity is characterized through the use of TPROGS (Carle, 1997;Carle and Fogg, 1996;Carle and Fogg, 1997). TPROGS is a structure imitating geostatistic method that has been applied successfully to aquifers dominated by sand/gravel in several cases units (Carle et al., 1998;Fogg et al., 1998;Weissmann et al., 1999;Weissmann and Fogg, 1999). In this manuscript it is investigated to what extent TPROGS can be used in characterization of aquifer heterogeneity when applied to a multi aquifer complex dominated by clayey till.

In application of TPROGS it was realized that, despite more than 1000 wells, the data material was too sparse to justify fitting a geostatistic model in other than vertical direction. Construction of a 3D Markov chain model for the Quaternary aquifer complex required additional information besides well logs, subjective knowledge in form of geological insight and interpretation of other data sources. Characterizing of this complex aquifer system through means of geostatistic methods involved a few steps of possible more general interest:

- Modeling of the entire area using a single 3D markov chain model could not be done without violating the stationarity condition. To overcome this, the area was split up into five zones of interpreted different depositional environment. Outlining of the zones were primarily based on geomorphological maps. This procedure of

subdividing an aquifer complex into units of apparent stationarity is in essence equivalent to traditional stratigraphic delineation. In a Quaternary aquifer complex it is, however, difficult to correlate stratigraphic units, especially throughout aquifers of regional extent. Secondly, we were interested in representing inter-aquifer heterogeneity, not heterogeneity of the individual aquifer units.

- The apparent mean lengths and directional tendencies of the major facies were interpreted from soil surface maps and cross-sectional analysis. The analysis of soil survey maps did not produce any obvious directional tendencies for sand/gravel or meltwater hydro-facies. A mean length of sand/gravel was determined to be between 1000-8000 meters and the mean length for meltwater clay was between 250-800 meters.
- Through Markov chain modeling it is possible to simulate juxtapositional tendencies, but the analysis of this aquifer complex did not suggest any juxtapositional tendencies between sand/gravel, meltwater clay and till.

From the Markov chain model 10 realizations of aquifer heterogeneity was established using TPROGS. The realizations were conditioned to well log data and the hydraulic parameters were calibrated inversely to head and discharge observations. Subsequent evaluation of the realizations was split up in a qualitative evaluation of cross sectional representation of geological heterogeneity and a parameter/calibration evaluation. Each of the realizations showed a geological representation that was in agreement with expected geological heterogeneity. Parameter-wise the calibrated values were in agreement with prior conceptualization for 7 out of 10 realizations.

Final calibration results show a minimized objective function value of same magnitude as the homogeneous case (similar to the simple conceptualization of manuscript two), some had smaller and some had larger residuals. Prediction analyses was carried out following the procedure of manuscript two and inter compared and compared with the deterministic simulations of the four different conceptualizations of manuscript two. Direct comparison of concentrations shows similar predictive capabilities for the stochastic simulations as for the deterministic simulations, with only minor improvement in the ability to encapsulate observations. Comparing simulated concentrations of environmental tracers, however, neglects the variations in the part of the simulated age distributions older than approximately 50 years – equal to the time span where environmental tracers have been present in the atmosphere as a consequence of human activity. Comparison of age distributions revealed large variation between stochastic and deterministic simulations.

# Conclusion and perspectives

Physically based modeling of regional scale aquifer complexes involves conceptualizing aquifer structures and assigning parameters in order to simulate observations. The present research has focused on simulation of groundwater flow and transport and the importance of aquifer conceptualization in this regard.

The simulations of age distribution in manuscript one seemed fairly insensitive to changes in parameters and in manuscript two and three sensitive to changes in conceptualization. This indicates that parameter manipulation is of less importance than model structure, when model simulations are extrapolated beyond calibration base. Present analytical methods that can relate tracer concentration and groundwater age from analytical descriptions of flow fields, hence the influence of geological heterogeneity is pre-determined by choice of analytical solution. It was demonstrated that there could be a problem related to this traditional method when applied to complex aquifer systems, but at the same time it was shown that environmental tracers could be used if certain precautions are taken. The present study has demonstrated the usefulness of environmental tracers for investigation of transport behavior, but has also shown that it is crucial, that environmental tracers are simulated in terms of concentrations instead of being re-interpreted into ages.

The modeling approach in all three manuscripts has been to calibrate the groundwater flow model (hydraulic conductivities) against groundwater head and discharge observations and then use these models in an extrapolation mode to predict groundwater transport behavior. A first conclusion from comparison of the transport simulations with observed tracer data is that the performance is quite modest. The conceptualizations that are good enough for groundwater flow simulations needs substantial improvement to be adequate for transport.

Based on 32 measurements of environmental tracers it was not possible to reject any of the 14 alternative models of manuscripts two and three. At the same time non of the simulations was able to accurately predict the measured concentrations of environmental tracers. The concentration ranges predicted by the different models were not able to encapsulate all the observations. Thus, even combined, the model simulations are likely to underestimate the uncertainty related to model structure in the investigated cases. It is likely that measurements of environmental tracers can aid in establishing an objective reference for discriminating between models. Two questions must be addressed prior to this. Firstly, tracer observations taken from

filters without pumping represent a limited volume compared to model scale. There is a need for investigations that can determine to what extent these point observations can be interpreted as volume measurements. Secondly, how many measurements of environmental tracers, spatial as well as temporal, do we need to get robust conceptualizations? Is the added value of extra tracer measurements comparable to the other types of information? We might be able to address this question through model studies of synthetic geological settings with synthetic information.

Simulations using alternative deterministic and stochastic models indicate that the conceptualization essentially affects our ability to produce predictive results. Many of the relative distinctive differences between the conceptual models were to some extent blurred by the calibration process, at least in the model ability to simulate calibration targets. This has consequences regarding the generality of any model: results from a model of one area cannot be transferred directly to another area, and simulation of subjects that are included in the calibration targets are apparently connected with a higher degree of certainty, certainty that might just as easy be misleading. It rises the question of whether it is at all possible to determine or delimit model uncertainty based on a parameter / calibration analysis. The concern is increased once model predictions are extrapolated from the calibration base.

The subjective nature of conceptualization, as demonstrated in manuscript two and three affects the objectivity for a given discrimination of conceptualizations. At the same time subjectivity is an integral part of conceptualization, even when geostatistical methods are applied. The subjectivity provides us with freedom to translate geological data to model-scale. We have shown several levels of generalizations of geological data. From the simple model of manuscript two where it is only the more general properties that is categorized, to the stochastic model that honors all geological data directly based on data quality. In manuscript two it is shown that is not wise to single out the conceptualization based on calibration performance alone, which is elsewhere presented as an acceptable procedure (Poeter and Hill, 1998). The increased knowledge gained by using more than one model is increasing the uncertainty range.

With increased uncertainty range it may be necessary to come up with methods that can discriminate between alternative conceptualizations. In this perspective agreements between certain conceptualization aspects (parameter-structures) and the final model might be of central importance. In this context it will be important to document decisions on processes, structures and assumptions during model construction. Even though there may be an infinite number of models that may be

suited for modeling of a scenario, there may be equally as many unsuitable. It is in this context the coherence between conceptualization, behavior and other types of knowledge will become important.

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