MODELING GROUNDWATER FLOW IN GEOLOGICAL COMPLEX AREAS USING LOCAL GRID REFINEMENT, COMBINED PARAMETERIZATION METHODS, AND JOINT INVERSION

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS OF THE PH.D. DEGREE

TROELS NORVIN VILHELMSEN

DEPARTMENT OF GEOSCIENCES
AARHUS UNIVERSITY
DENMARK
SEPTEMBER, 2012
This thesis entitled: "Modeling groundwater flow in geological complex areas using local grid refinement, combined parameterization methods and joint inversion" is written as partial fulfillment of the requirements of a three year Ph.D. (doctor philosophiae) program, during an enrollment at the Department of Geoscience, Aarhus University. The work was conducted under the supervision of Assoc. Prof. Steen Christensen and it was financed by the Danish Council for Strategic Research and Aarhus Vand A/S through the HYdrological Modelling for Assessing Climate Change Impacts at different Scales (HYACINTS) project (www.hyacints.dk). The thesis includes a paper written in corporation with Assoc. Prof. Steffen W. Mehl of CSU, Chico, and United States Geological Survey (USGS), Boulder CO. The work presented in this paper was initiated during a short stay at USGS, Boulder, CO visiting Senior Research Hydrologist Mary C. Hill.

The work conducted during this Ph.D. is presented in this thesis and it comprises three scientific manuscripts, where one has been published in an international Journal while the others are almost ready for submission (see list below). Moreover, the work includes various presentations given at workshops, international and national conferences; teaching activities; and Ph.D. courses. These last contributions are only presented in list form with name and location.

**Paper 1:** Vilhelmsen, T.N., Christensen, S., Mehl, S.W., 2012, *Evaluation of MODFLOW-LGR in Connection with a Synthetic Regional-Scale Model*, Ground Water, 50, 1, 118-132


Presentations, abstracts, teaching and Ph.D courses

Presentations:
Poster presentation: AGU Fall Meeting 2009, San Francisco, U.S.A
Poster and oral presentation: ATV Winter Meeting 2010, Vejle, Denmark
Poster presentation: AGU Fall Meeting 2011, San Francisco, U.S.A
Various oral presentations at steering committee meetings, Ph.D meetings and Ph.D courses

Abstracts and proceedings:

Vilhelmsen, T.N., Christensen, S., Test af to versioner af MODFLOW-LGR til simulerings af grundvandsstrømninger i omrider med begravede dale – syntetisk studie, ATV vintermøde 2010, Vejle, Denmark, 5-7 February 2010 (in Danish)


Teaching:
In total 840 hours of teaching has been given during this Ph.D. project within the following topics: Groundwater modeling and geostatistics at Ms.C. level; Field courses mainly within performance and analysis of slug tests, collection of hydraulic head data and stream flow measurements; and finally teaching at High School level within climate change

Ph.D. courses:
Introduction to programming, Dep. of Computer Science Aarhus University, Denmark (5 ECTS)
Numerical solutions to partial differential equations, Dep. of Computer Science Aarhus University, Denmark (5 ECTS)
Geostatistics and GIS, Faculty of Agricultural Science, Aarhus University, Denmark (5 ECTS)
Uncertainty in Environmental modeling, Uppsala University, Uppsala, Sweden (5 ECTS)
Modeling of Heterogeneity and Transport in Geologic Media, FIVA, International Research School of Water resources, University of Copenhagen, Denmark (6 ECTS)
Academic English, Aarhus University, Denmark (3 ECTS)
Surface-ground water interaction: From watershed processes to hyporheic exchange FIVA, International Research School of Water resources, University of Copenhagen, Denmark (5 ECTS)
Acknowledgements

In the course of a Ph.D. study several have people been involved to more or less degree. By naming individuals you always bear the risk of forgetting someone, this has not been done out of bad intentions but more from a stressful mind in the final stages of this work.

First, I would like to acknowledge the assistance of my supervisor Steen Christensen. You have given me academic as well as personal support during these years. Your guidance in academic issues has been greatly appreciated. You seem to have endless personal resources always lending an ear of personal issues. This is an inspiration.

A major gratitude goes to my in-laws. Without your endless support during these year I would not have come this far. You help my wife and me tremendously in our daily life, and your assistance is more appreciated than you could ever comprehend. A special thanks goes to my mother-in-law. You have a tight bond with my son, which is created through the many hours you spend with him. Without you help to take care of him during sickness, we would not have been able to mind of our jobs. In the final stage of this Ph.D. you lived with us to take care of us and him. Without this help my thesis would not have been handed at the time it did.

Without the love and support of my wife this work had not been finished. You brought me back to reality when things where overwhelming. These stressful years have been tough on both of us, and I hope and believe that they have left me stronger.

My son helps to bring things into perspective; you bring a smile to my face even at the toughest days.

Finally, I would like to acknowledge my friends, fellow Ph.D. student, colleagues and family. Especially Steffen Mehl and Mary Hill; I had a great but short stay Boulder and I hope to be able to go there again someday.

The Ph.D. project was financed by the Danish Council for Strategic Research and by Aarhus Vand A/S through the HYACINTS project. I greatly appreciate the support, and I hope that the results presented can be of use for practitioners and further scientific research.
# Table of Content

- Preface ........................................................................................................... I
- Presentations, abstracts, teaching and Ph.D courses ........................................ II
- Acknowledgements ........................................................................................... III
- English summary ................................................................................................. 1
- Dansk sammenfatning ........................................................................................ 3
- List of figures ....................................................................................................... 5
- Introduction ......................................................................................................... 6
- 1 Flow of groundwater in porous media ............................................................ 8
  - 1.1 Mathematical description of groundwater flow ......................................... 8
  - 1.2 The finite difference method applied to groundwater flow problems .... 8
  - 1.3 Local grid refinement methods for finite difference solutions ................. 10
- 2 Inversion of numerical models ....................................................................... 14
  - 2.1 Least squares inversion of nonlinear models .......................................... 14
    - 2.1.1 Damping ............................................................................................. 15
    - 2.1.2 Scaling ............................................................................................... 16
    - 2.1.3 The Levenberg-Marquardt method .................................................... 16
    - 2.1.4 Data weighting and model errors ...................................................... 17
  - 2.2 Stabilizing ill-conditioned or singular inverse problems ......................... 17
    - 2.2.1 Tikhonov Regularization ................................................................... 18
    - 2.2.2 Singular Value Decomposition (SVD) ............................................ 19
    - 2.2.3 Reducing dimensionality through SVD-assisted inversion ............. 20
  - 2.3 Joint inversion ............................................................................................ 21
    - 2.3.1 Inversion using multiple data types .................................................. 21
    - 2.3.2 Linking models in the inversion process ......................................... 21
- 3 Parameterization ............................................................................................. 25
  - 3.1 The principle of parameter parsimony ..................................................... 25
  - 3.2 Parameterization using zones ..................................................................... 26
  - 3.3 Parameterization using pilot points ......................................................... 26
  - 3.4 Combining pilot points with zones ........................................................... 27
  - 3.5 Applying an upscaled geological model to the numerical model ........... 28
- 4 Burried Quartenary valleys and their importance for groundwater groundwater resources ........................................................................................................... 30
  - 4.1 Structure and origin .................................................................................... 30
  - 4.2 Mapping ..................................................................................................... 30
This thesis deals with local grid refinement (LGR) as a methodology of downscaling hydrological models and to incorporate geological complexity into a regional scale groundwater model. Moreover, it documents two methodologies to perform joint inversion between geophysical data and groundwater models. In the present case it is used to couple a two dimensional numerical model having cylindrical geometry used for aquifer test analysis to two geophysical models. However, the primary perspective is to apply the method for full three dimensional joint inversion of geophysical and hydrological data sets.

A thorough analysis of the iterative MODFLOW-LGR method documents the benefits and drawbacks of this methodology. It is shown that by applying LGR it is possible to increase the local simulation accuracy of a regional scale model that otherwise uses a coarse numerical discretization. Moreover, it is shown that LGR of the numerical grid makes it possible to also increase the geological resolution used in the model without affecting its simulation efficiency. Some limitations are documented as well. It is shown that the iterative coupling can lead to runtimes that are longer than for a model using a globally fine grid. For the presented case it is found that the locally refined part of the model should not comprise more than 10-15% of the total model domain; otherwise global refinement is superior. However, this limitation will be influenced by the variation in the hydraulic conductivity field. This is documented through an analysis of how model runtimes for LGR and a globally refined model depend on the coefficient matrix condition number. This shows that the iterative LGR methodology tends to suffer more from high condition numbers than the equivalent model using a globally refined grid. This reduces the efficiency of the iterative coupling.

The MODFLOW-LGR method is also applied to a regional scale field site model. Here it is utilized to increase the numerical and the geological resolution in the vicinity of a newly established well field extracting groundwater from a buried valley structure. The LGR method is in this case combined with the use of an up-scaled geological model and pilot points to increase the hydraulic conductivity resolution within the focus area of the model domain. Some of the results obtained in this study are in good agreement with those described above, namely that the numerical resolution of a groundwater model seems to have a larger impact on model calibration and prediction accuracy than the geological resolution. For the field case this is evident since locally refined models having fine and coarse geological resolution, respectively, produced similar fits to the calibration dataset. However, when using these models to predict the impact from the well field the model with the finer geological resolution performed better than the one with the coarse geological resolution. The use of pilot points allowed for estimation of heterogeneity within the buried valley structure. It is shown that the same overall heterogeneity structure is estimated no matter the calibration dataset applied, but there are small scale differences. By using the calibrated models for prediction it is shown that the small scale differences can have a large influence on model predictions. This indicates that further constraints are needed on the pilot points in order to achieve a unique solution. It was the intention to establish such constraints by joint inversion using local transient electromagnetic (TEM) soundings. However, the available TEM data from the area was not of sufficient quality to perform such an analysis. A method to perform similar constraints was however tested in this study using magnetic resonance data and TEM soundings. This is described in the following.

The final study develops and tests two methods of joint inversion of hydrological and geophysical datasets. The coupling is performed using an empirical petrophysical relation between geophysical parameters and hydraulic conductivity. By analyzing the methodology using a synthetically generated model it is shown that accurate estimates can be obtained for geophysical and hydraulic parameters as well as empirical prefactors pertaining to the petrophysical relation. Using the methodology detailed estimation can be obtained also at depths that are not reached by wells and boreholes. A similar joint inversion methodology could be used to better constrain the hydraulic conductivity field described in the
previous study. Applying it in a complex three dimensional environment does, however, require more development and testing.
Dansk sammenfatning


I det sidste studie er der dokumenteret og anvendt en samlet inversion af geofysiske data simuleret ved brug af geofysiske modeller og prøvepumpningsdata simuleret ved brug af en numerisk grundvandsmodel. Koblingen sker ved anvendelse af en empirisk relation mellem geofysiske parametre og hydrologisk ledningsevne. Metoden er testet ved anvendelse af en syntetisk model bestående af to grundvandsmagasiner separeret af et lerlag, hvor kun det øvre magasin er moniteret under prøvepumpningen. Herved er det dokumenteret, at der kan opnås detaljerede estimatorer af såvel
hydrauliske som geofysiske parametre. Den samlede inversion har desuden potentiæle til anvendelse i tredimensionelle grundvandsmodeller til beskrivelse af den rumlige variation i hydraulisk ledningsevne. Dette vil dog kræve yderligere undersøgelse og tests.
## List of figures

Figure 1-1: Setup used for the normal block centered finite difference formulation describing the flow from the six surrounding cells to the center cell (after McDonald and Harbaugh 1988). ........................................... 9

Figure 1-2: Schematic description of different types of two dimensional finite grids. Grids are shown for the traditional finite difference formulation presented in the previous section, a one way coupling between a local grid and a coarse scale grid and finally an unstructured grid where a coarse scale grid has an embedded local scale grid. ................................................................. 11

Figure 2-1: Joint inversion of a groundwater model and a geophysical model using method 1. Multiple geophysical models can be added to this setup using the same or different petrophysical relations. ....... 22

Figure 2-2: Joint inversion using of a groundwater model and a geophysical model method 2. Multiple geophysical models can be added to this setup using the same or different petrophysical relations........ 23

Figure 3-1: Example of a hydraulic conductivity field created by a combination of pilot points and zones of piecewise constant values. In the hatched area, parameter values are defined through zones. This area comprises low permeable clays which the buried valleys (the un-hatched area) are incised into, and some sand units. In the unhatched area variation in hydraulic conductivity is defined through pilot points. Here a smooth variation is seen, which is meant to describe a diluvial environment. .............................................. 27

Figure 3-2: Schematic description of a voxel based geological model (left) and the principle of the upscaling methodology (right) used for creating input to the numerical groundwater model. .......... 28

Figure 4-1: Description of data coverage and buried valleys located in the Aarhus Nord area which is the primary focus area of this thesis, and the area analyzed in paper 2. The buried valley structures shown on the figure are based on the descriptions of Jørgensen and Sandersen (2009b) ........................................ 32

Figure 5-2: Cross sections showing the differences in geological resolution used for comparing the importance for the geological resolution of the model .................................................. 33

Figure 5-1: Schematic description of the terrain and the bottom of the buried valley (top of the green cells in Figure 5-2). The square shows the locally refined area. The cross sections shown on Figure 5-2 only cover this area ................................................................. 33

Figure 5-3: Simulation errors comparing the locally refined model with a numerical model having the numerical resolution of the parent model over the entire domain ........................................ 34

Figure 5-4: Errors in heads in a horizontal cross section through the LGR models. The black lines indicate the edges of the valley structure. It is evident that locally around heterogeneities large errors are introduced using a flawed geological resolution ........................................ 34

Figure 6-1: The field site used in the analysis, showing the location of the regional scale model and the locally refined models ................................................................. 36

Figure 6-2: Example of simulations from two boreholes comparing the locally (right) and regionally (left) calibrated models ................................................................. 37

Figure 6-3: Drawdown simulations from one of the four observation wells ........................................ 38

Figure 6-4: Validation results for two selected boreholes comparing results from the regionally and the locally calibrated models ................................................................. 39

Figure 6-5: Calibrated hydraulic conductivity fields for the LGR models with a refined valley resolution, calibrated either to head data (left) or both head data and aquifer test data (right) ........................................ 40

Figure 7-1: Estimated parameter values using the joint inversion methodology ........................................ 41

Figure 7-2: Methodology for coupling aquifer test data with MRS data using a smooth/many layer model... 42
Introduction

This Ph.D. project is a part of the HYdrological Modelling for Assessing Climate Change Impacts at different Scales (HYACINTS) project (www.hyacints.dk) which is a five year research project initiated in 2008. The main objective of this research project was to develop new methodologies and tools to enable easier and more accurate use of regional scale climate and hydrological models to address local scale water resource problems. The topics covered by the HYACINTS project spans widely from climate modeling, conceptual model uncertainty, including complex geology in groundwater models, and downscaling of hydrological simulations. However, they all address the same issue: how to achieve reliable model predictions of local water resource problems under changing climatic conditions.

The main motivation is driven by the effects of climate change on local scale water resource problems. Several studies have shown that a changing climate can have a profound effect on regional scale water resources (Andréasson et al. 2004; Caballero et al. 2007; Graham et al. 2007; Thodsen 2007; van Roosmalen et al. 2009). However, in some areas the flow of groundwater cannot be simulated accurately using the coarse numerical discretization of a regional scale groundwater model due to the complexity of the local scale geological environment. In such cases effective methods for refining the regional scale models need to be investigated. Some numerical methods have an inherent and thereby more easily applied method for performing local refinement in the horizontal plane than others. This typically accounts for finite-element codes like FEFLOW (Diersch 2002). Grid refinement methods have also been developed for finite-difference models, using either the integrated finite-difference approach (De Marsily et al. 1978; Edwards 1996), or the point centered approach (Jackson and A.E.F. 1999; von Rosenberg 1982). Both these methods use unstructured grids which compromise the traditional and well ordered finite difference stencil, making the system harder to solve. An alternative to this is the embedded approach; here two or more models are coupled through boundary conditions located at the interface between the locally refined model and the regional scale model (Leake et al. 1998; Mehl and Hill 2002; Mehl and Hill 2004; Mehl and Hill 2005; Szekely 1998). This method has the benefit that the well ordered finite difference system of equations is kept, hereby rendering the use of effective solvers. Through local grid refinement the complexity of the local geological environment can be better incorporated into regional scale groundwater models, without compromising the accurate description and the dynamics of the outer boundary conditions affecting local scale predictions.

Local grid refinement has been utilized in several studies to increase the numerical resolution locally within regional scale groundwater models (Davison and Lerner 2000; Gurwin and Lubczynski 2004; Hunt et al. 2001). One of the challenges of applying local grid refinement lies in the automated parameter estimation process. Changes to parameter values, whether they cross the interface between the local and the regional model or not, need to be implemented in both models in order to achieve accurate boundary conditions at the interface. Davison and Lerner (2000) acknowledged this by first introducing changes in their regional scale model and subsequently updating the local scale model, and Gurwin and Lubczynski (2004) incorporated it indirectly by calibrating general head boundary conductances estimated based on a regional model. However, in order to conduct a fully automated parameter estimation process the regional and the local models need to be closely linked and updated simultaneously in the parameter estimation process. This can be accomplished by utilizing the MODFLOW-LGR (Mehl and Hill 2005) model. Here models are closely linked, and interface boundary conditions are thereby updated automatically either using a one way coupling or an iterative process. The latter results in a more accurate solution.

The increased numerical resolution of a locally refined model can be utilized to increase the geological resolution of the model. This can be done in order to obtain a more accurate description of known interfaces between geological units. The increased numerical resolution can also be used to achieve a
more accurate interpolation of a smoothly varying field interpolated using the pilot point method (Certes and De Marsily 1991; Doherty 2003). Utilizing pilot points for describing smooth variations in aquifers has benefits and drawbacks. Compared to zones the methodology results in aesthetically pleasing hydraulic conductivity fields, especially when analyzing sediments deposited through fluvial processes. This type of depositional environment is expected to vary smoothly, which conflicts with the traditional parameterization using zones of piecewise consistency. However, the pilot point method is often criticized for resulting in an over parameterized model which conflicts with the principle of parameter parsimony. See e.g. Hill (2006) who has a detailed discussion of this topic. In order to stabilize the inversion process regularization constraints are often imposed on pilot point values (e.g. Doherty 2003; Tonkin and Doherty 2005). Depending on the inversion setup and data availability the regularization constraints can be formed in different ways. A typical method employed is the smoothing constraint where closely positioned pilot points are expected to be more similar than more distant ones. However, a more robust methodology could potentially be to link these estimates of pilot point values to geophysical measurements or similar densely sampled data reflecting the heterogeneity of what is modelled by the pilot points.

This thesis deals with some of the topics described above. In total it comprise this resume, which in detail describes the methods applied to the problems analyzed and gives a short resume of the papers written. The three papers deals with the following topics. The first paper gives a thorough analysis of the MODFLOW-LGR method in order to determine its capabilities for applying local grid refinement within an area dominated by buried valley structures. The second paper describes a study where the local grid refinement method has been utilized to analyze the importance of numerical and geological resolution and calibration datasets when making predictions of local scale water resource problems in an area with a complex geological setting. The final paper presents a novel method for performing joint inversion between datasets from the transient electromagnetic method (TEM), the magnetic resonance sounding (MRS) method, and aquifer tests. Here the method is presented using a numerical two dimensional groundwater model, but potentially it can be applied to a full three dimensional groundwater model to constrain pilot point values to stabilize the inversion problem.

The thesis is organized as follows. First the general theory for flow of groundwater in porous median is described together with different forms of finite difference solutions for the three dimensional diffusion equation. Second, the general theory is described for inversion of numerical models using the least squares method using various forms of regularization. Third, methodologies for parameterization of numerical models is discussed, mainly with focus on spatial representation of hydraulic conductivities. Fourth, a short description of buried valley structures, their occurrence and morphology is given with main focus on their importance for groundwater flow. Fifth, short resumes are given of each paper written as support for the thesis, and references will be given to the theories described. Finally conclusions are drawn based on the conducted work, and perspectives are given relating to future scientific work.
1 Flow of groundwater in porous media

1.1 Mathematical description of groundwater flow

The flow of groundwater in a porous medium can be described by the diffusion equation derived from Darcys Law (Darcy 1856) and the law of conservation of mass:

\[ \text{div}(K \ast \text{grad} \,(h)) - w = S_s \frac{\partial h}{\partial t} \]  \hspace{1cm} (1.1)

where \( K \) is the hydraulic conductivity tensor, \( h \) is the groundwater head, \( w \) is a source/sink term, which might be head dependent, \( S_s \) denotes the specific storage of a confined aquifer, and \( t \) is time. Assumptions used for deriving (1.1) can be found in most textbooks on groundwater hydraulics e.g. Bear (1979, p. 92-93).

In the special case where the medium analyzed is anisotropic and heterogeneous, and the principal directions of the system analyzed is located in the \( x, y, \) and \( z \) directions, (1.1) can be reformulated to

\[ \frac{\partial}{\partial x} \left( K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial h}{\partial z} \right) - w = S_s \frac{\partial h}{\partial t} \]  \hspace{1cm} (1.2)

In order to get a unique solution of (1.2) initial and boundary conditions need to be applied. The initial conditions are given as

\[ h(x, 0) = h_0(x, 0) \]  \hspace{1cm} (1.3)

Depending on the model setup and the simulations performed several different boundary conditions approximating different conditions can be used. These can be summarized as

\[ \alpha \ast h(x, t) - \beta \ast \text{grad}(h) = C(x, t) \]  \hspace{1cm} (1.4)

If \( \alpha = 1 \) and \( \beta = 0 \) a Dirichlet boundary condition is applied; if \( \alpha = 0 \) and \( \beta = 1 \) a Neumann boundary condition is applied; and if \( \alpha = 1 \) and \( \beta = 1 \) a Cauchy boundary condition is applied (Bear 1979, pp. 96-98; de Marsily 1986, pp. 135-141; Østerby 2008, pp. 3-4). When analyzing groundwater problems these three types of boundary conditions can be exemplified as follows:

- First kind (Dirichlet): this type of boundary condition would in a groundwater model be used to describe a prescribed/constant head
- Second kind (Neumann): this type of boundary condition could be either a no-flow boundary \([C(x, t) = 0]\) or a specified flux boundary \([C(x, t) = q]\) e.g. a well
- Third kind (Cauchy): This type of boundary condition describes a head dependent flow condition. This is typically used to represent groundwater streamflow interaction or simulation of drains

1.2 The finite difference method applied to groundwater flow problems

For relatively simple systems analytical solutions to (1.1) and (1.2) can be derived under constraints imposed by (1.3) and (1.4). However, for more complicated systems numerical methods provide the only solution. The work presented in this thesis is based on the finite difference solution to (1.2) but other solution methods such as the finite element method or the finite volume method could have been applied as well.
Finite difference approximations to (1.2) can be derived in different ways, which all result in the same solution. Through expansion of the derivatives in (1.2) using a truncated Taylor expansion the finite difference approximation can be obtained together with a truncation limit (Bear 1979, pp. 131-134). However, a more simple method is to describe the system by applying Darcy’s Law to a small portion of the model domain (see Figure 1-1).

![Figure 1-1: Setup used for the normal block centered finite difference formulation describing the flow from the six surrounding cells to the center cell (after McDonald and Harbaugh 1988).](image)

By setting up the system on a 3 dimensional Cartesian grid the rate of flow from the left hand side cell into \( p_{(r,c,b)} \) can be determined by

\[
q_{(r,c-\frac{1}{2},0)} = C_{(r,c-\frac{1}{2},1)} \ast \left( h_{(r,c-1,0)} - h_{(r,c,1)} \right)
\]

where \( r, c, l \) are the row, column and layer respectively; \( C_{r,c-1/2,l} \) denotes the conductance between cell \( p_{(r,c,l)} \) and the left hand side cell; \( q_{r,c-\frac{1}{2},l} \) denote the amount of water flowing from the left hand side into the present cell, and \( h_{r,c-1,l} \) and \( h_{r,c,l} \) denotes the heads in the two cells. Similar equations can be set up for all adjacent cells resulting in a mass balance term stating that the sum of water entering and leaving the cell is equal to the change in water storage with time.

\[
\sum_{i=1}^{n} q_i = S_s \ast \frac{\Delta h}{\Delta t} \ast \Delta V
\]

The right hand side sums the flow into and out of the cell, \( \Delta h \) is the change in hydraulic head, \( \Delta t \) is the timestep, and \( \Delta V \) is the volume of the cell (McDonald and Harbaugh 1988)
By combining the terms given by (1.5) for all cell faces pertaining to cell \( p_{(r,l,c)} \) in Figure 1-1 the finite difference equation can be formulated as

\[
q_{(r,c-\frac{1}{2},l)} + q_{(r,c+\frac{1}{2},l)} + q_{(r-\frac{1}{2},c,l)} + q_{(r+\frac{1}{2},c,l)} + q_{(r,c,l-\frac{1}{2})} + q_{(r,c,l+\frac{1}{2})} + w_{(r,c,l)} = S_{s_{(r,c,l)}} * \Delta h / \Delta t * \Delta x * \Delta y * \Delta z \Rightarrow \\
C_{(r,c-\frac{1}{2},l)} * \left( h_{(r,c-1,l)}^m - h_{(r,c,l)}^m \right) + C_{(r,c+\frac{1}{2},l)} * \left( h_{(r,c+1,l)}^m - h_{(r,c,l)}^m \right) \\
+ C_{(r-\frac{1}{2},c,l)} * \left( h_{(r-1,c,l)}^m - h_{(r,c,l)}^m \right) + C_{(r+\frac{1}{2},c,l)} * \left( h_{(r+1,c,l)}^m - h_{(r,c,l)}^m \right) \\
+ C_{(r,c,l-\frac{1}{2})} * \left( h_{(r,c,l-1)}^m - h_{(r,c,l)}^m \right) + C_{(r,c,l+\frac{1}{2})} * \left( h_{(r,c,l+1)}^m - h_{(r,c,l)}^m \right) \\
+ w_{(r,c,l)} = S_{s_{(r,c,l)}} * \frac{h_{(r,c,l)}^m - h_{(r,c,l)}^{m-1}}{\ell^m - \ell^{m-1}} * \Delta x * \Delta y * \Delta z
\]

(1.7) is formulated using the implicit finite difference method, where \( m \) denotes the present time step resulting in one equation with seven unknowns for each cell in the grid. It is readily apparent that (1.7) cannot be solved since it holds more than one unknown. However, when formulating similar equations for every cell in the grid the modeler is left with the same number of unknowns and equations as the number of cells in the grid.

By rearranging (1.7) for all cells in the grid and isolating unknown head values together with their coefficients on the left hand side and known heads and source/sink terms on the right hand side the combined system of equations can be written on matrix form as

\[
A h = d
\] 1.8

where \( A \) is a matrix holding the coefficients derived from the conductance terms and head dependent boundary conditions, \( h \) is a vector holding unknown heads estimated at the end of the present time step, and \( d \) is a vector holding constant terms derived from boundary conditions and known heads. This methodology for deriving the finite difference set of equations is the one used in the documentation of the U.S. Geological Survey groundwater flow model code MODFLOW (Harbaugh 2005; Harbaugh et al. 2000; McDonald and Harbaugh 1988; Mehl and Hill 2005).

When the system of equations is well ordered as is the case for the system presented above the coefficient matrix has a fixed structure with nonzero elements only in the diagonal and six off-diagonals, three above and three below the main diagonal. This fixed structure allows the development of fast highly effective solvers. For MODFLOW these include for example the Preconditioned Conjugate-Gradient (PCG) solver (Hill 1990), and the GMG Linear Equation Solver (Wilson and Naff 2004).

1.3 Local grid refinement methods for finite difference solutions

Locally refined finite difference models can be utilized to describe subareas of a specific model domain in more detail. This could either be in order to make accurate simulation of contaminant transport (Davison and Lerner 2000), make accurate simulations of groundwater-stream interactions (Mehl and Hill 2010) or to better resolve geological features (Vilhelmsen et al. 2012). Local grid refinement can either be applied as a direct refinement of the numerical grid (de Marsily 1986, p. 351; Edwards 1996; Jackson 2001; von Rosenberg 1982), or through boundary conditions linking a local scale model to a regional scale model either using one way coupling (Leake and Claar 1999; Leake et al. 1998) or iterative coupling (Dickinson et al. 2007; Mehl and Hill 2001; Mehl and Hill 2002; Mehl and Hill 2004; Szekely 1998). A schematic description of these three types of couplings are given for a two dimensional grid in Figure 1-2.
By solving the traditional two dimensional finite difference system of equations for the grid presented in Figure 1-2 using the method presented in section 1.2, equation (1.8) takes the form

\[
\begin{bmatrix}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{bmatrix}
\begin{bmatrix}
h_1 \\
h_2 \\
h_3 \\
h_4 \\
h_5 \\
h_6 \\
h_7 \\
h_8 \\
h_9
\end{bmatrix}
= d
\]

In order to make the formulation general, non-null values of the coefficient matrix \( A \) has been substituted by black squares, and null values have been left empty. For the two dimensional case each head value is dependent on the adjacent four cells. The coefficient matrix in (1.9) therefore has a maximum of four off-diagonal elements located in a fixed structure.

A similar fixed structure is achieved using the one-way (TMR) or the iterative (LGR) coupling shown on Figure 1-2. Here models are linked through boundary conditions imposed by one grid structure on the other. For the one-way coupling Dirichlet or Neumann boundary conditions are often used for defining boundary conditions for the local scale model (Leake et al. 1998; Mehl et al. 2006), where Dirichlet boundary conditions often provides the most accurate results (Mehl et al. 2006). For the LGR coupling boundary conditions at the interface between the two models are balanced iteratively until a specific stop criterion is met. For such a coupling constant Dirichlet boundary conditions are often imposed on the local scale model based on results from the coarse scale model while Neumann boundary conditions are often imposed on the coarse scale model based on the local scale model (Mehl and Hill 2002; Szekely 1998).
The combined system of equations for the TMR or the LGR coupling can be seen from (1.10). This equation setup does however first apply for the second iteration since the coarse scale model must be run for the entire domain during the initial simulation. For the second iteration, the part of the coarse scale model completely covered by the local scale model must be excluded from the simulation through a no-flow condition. This can be achieved by zeroing out the rows and columns of the corresponding no-flow cell and setting the corresponding main diagonal element in $A$ equal to one.

Comparing the LGR method to the TMR method Mehl and Hill (2002; 2004) found that the TMR method might result in less accurate solutions due to the lack of feedback to the coarse scale model. However, this feedback comes at a price. By increasing the hydraulic conductivity contrast between units in the groundwater model the condition number of the coefficient matrix increases. As a natural consequence of this the runtime and number of iterations for the LGR method increases (Mehl and Hill 2002; Vilhelmsen et al. 2012). This accounts for both regionally refined models and LGR models. However in some cases it might result in model runtime for the LGR model which exceeds that of a regionally refined model simulating the same system (Vilhelmsen et al. 2012). Other arguments besides model runtime might advocate for the application of the LGR method. In many cases local scale investigation areas might be located within already existing regional scale groundwater models (e.g. paper 2). In such cases the regional scale model can be utilized to generate accurate boundary conditions for the local scale model without making alterations to its structure. A slightly increased runtime can therefore be accepted, since it compensates for the potentially time consuming manual work to increase the numerical resolution of a regional scale model and updating its boundary conditions.
An alternative to the TMR or the LGR method is to apply the changes directly to the finite difference grid. This setup is named unstructured in Figure 1-2. The name refers to the fact that the well ordered finite difference stencil described above is compromised. For the case presented in Figure 1-2 the system of equations will take the following form

\[
\begin{bmatrix}
\vdots \\
\vdots
\end{bmatrix}
\begin{bmatrix}
h_{US1} \\
h_{US2} \\
\vdots \\
h_{US17}
\end{bmatrix} = d_{US}
\]

The coefficient matrix shown in (1.11) will however change appearance depending on the refinement ratio between the local and the coarse scale model, rendering the use of numerical solvers designed for a specific grid structure (like the ones presented above). Moreover, when applying the unstructured grid approach to the block centered finite difference grid conductance terms become more difficult to estimate. Dickinson et al. (2007) provides a method for calculating such conductances using ghost-nodes. However, in their case they use this coupling to link models using an iterative method, and not on an unstructured grid.

For the studies presented in this thesis it has therefore been chosen to use the LGR and the TMR methods. These methodologies have been utilized in paper 1 and paper 2 to test local grid refinement in a synthetic groundwater model and in a regional scale model used to perform detailed simulations around a newly established well field located in a buried valley structure.
When setting up a groundwater model the modeler must supply it with an initial set of parameter values \( \mathbf{p} \). These parameters will typically comprise hydraulic conductivities, specific yield, specific storage, streambed and drain conductances etc. Initial values for these parameters will be chosen from prior knowledge about the system or from hydrological investigations. However, the initial guesses will often be insufficient to make simulations which fit the calibration dataset. Manual calibration has frequently been used for adjusting the model parameters in order to achieve a good fit to the observation data. However, for complex models with multiple parameters, and especially for highly parameterized models, manual calibration is at best difficult and very time consuming and at worst impossible in practice. In such cases it can be beneficial to use auto-calibration, or inversion, to estimate model parameter values that make the model fit the observation data. In this chapter, the theory behind nonlinear inversion based on the least squares or Gauss-Newton method is presented. The chapter builds on the methodologies implemented in the independent parameter estimation software PEST (Doherty 2010).

### 2.1 Least squares inversion of nonlinear models

References covering the theory of nonlinear inversion are several, a few examples are: Aster et al. (2005); Cooley and Naff (1990); Doherty (2010); (Hill 1998). The basic theory for nonlinear inversion is the same as for linear inversion. The modeler wishes to find the set of parameter values which for example minimizes the sum of squared errors weighted by their inverse measurement standard deviation (Aster et al. 2005, p. 174). The relation between a nonlinear model and a set of observation data can be given as

\[
\mathbf{y} = f(\mathbf{x}, \mathbf{p}) + \mathbf{e}
\]

where \( \mathbf{y} \) holds the observation data; \( f(\mathbf{x}, \mathbf{p}) \) is the model describing the relation between the independent variables \( \mathbf{x} \), the model parameters \( \mathbf{p} \), and the observation data; finally, \( \mathbf{e} \) describes the misfit or residuals between model simulations and observed equivalents (Cooley and Naff 1990, p. 61). For simplicity, the independent variables are excluded in the following. The residual sum of squares can be written as

\[
\Phi = \mathbf{e}^T \mathbf{w} \mathbf{e}
\]

where \( \mathbf{w} \) is a weight matrix ideally depending on the covariance of the observation errors, or on the modelers desire to fit specific observations more accurately than others (Cooley and Naff 1990, p. 53). Moreover, when inverting models with multiple types of data, the weight matrix should be used to scale and adjust observation values so they produce comparable results. Otherwise minimizing (2.2) would produce meaningless results or mean that the model will only be fitted to certain parts of the calibration data. The weight matrix can either be a full or a diagonal matrix depending on whether observation errors can be assumed to be dependent or independent, respectively. However, sometimes using a full weight matrix will have limited effect on the inversion (Christensen et al. 1998).

When the model analyzed is linear, the optimal set of parameters minimizing (2.2) can be achieved in a single step. This is not achievable when the model is nonlinear. Instead a linear approximation to \( f(\mathbf{p}) \) is estimated using Taylor’s theorem (Cooley and Naff 1990, p. 61; Doherty 2010, p. 2-6)

\[
f(\mathbf{p}) \approx f(\mathbf{p}_0) + \mathbf{X}_0 (\mathbf{p} - \mathbf{p}_0)
\]

where \( \mathbf{X}_0 \) is the Jacobian or the sensitivity matrix computed using the initial parameters given as
Each term of the Jacobian matrix \( \frac{\partial f_k(p)}{\partial p_l} \) gives the sensitivity of the simulation of observation \( k \) to changes in parameter \( l \). Each column of the Jacobian matrix thereby holds information about the dependence of the observation dataset on the corresponding model parameters.

By inserting (2.3) and (2.1) into (2.2) the following term is achieved for the initial model misfit

\[
\Phi = e^T \omega e \approx [y - f(p_0) - X_0(p - p_0)]^T \omega [y - f(p_0) - X_0(p - p_0)]
\]

The minimum of the objective function is defined by the set of parameters for which the derivatives with respect to all parameters are zero. The parameter upgrade vector \( \Delta p = p - p_0 \) can therefore be determined by differentiating (2.5) and setting it equal to zero. After rearrangement the parameter upgrade vector for the first iteration can be determined as

\[
\Delta p = [X_0^T \omega X_0]^{-1} X_0^T \omega r
\]

where \( r = y - f(p_0) \) are the residuals between the observation data and equivalent model simulations using the initial set of parameter, \( p_0 \). By adding the parameter upgrade vector \( \Delta p \) to the parameter set \( p_0 \) a new set of parameter values is achieved which in principle should be closer than \( p_0 \) at minimizing (2.2). These are inserted into 2.3 and the process is repeated until the minimum of (2.2) is reached. This can be written as an iterative process giving \( p_{i+1} = p_i + \Delta p \). When no further improvement in the minimization of the objective function can be obtained by changing \( p_i \), the iteration process stops and the optimal parameter set \( \hat{p} \) has been found. Hopefully, this set of parameter values represents the global, and not just a local minimum of the objective function.

The elements of the Jacobian matrix \( X \), (note that \( X_0 \) has been substituted by \( X \) since \( X_0 \) represented the initial state of the system), must be calculated before a new iteration can be commenced. This part of the nonlinear inversion process is normally the most time consuming. The elements of the Jacobian matrix can be determined by solving the sensitivity equations; this is the methodology applied in MODFLOW-2000 (Hill et al. 2000). However, sensitivities can also be estimated by using perturbation methods. The benefit of this is that the inversion software can be developed to be model independent, since the elements of \( X \) can be approximated by finite differences. Estimating each column of \( X \) requires two (or more) successive model runs using different parameter values. This methodology is the one implemented in model independent inversion codes such as UCODE2005 (Poeter et al. 2005) and PEST (Doherty 2010).

2.1.1 Damping

Since the Gauss-Newton method builds on a linear approximation the length of \( \Delta p \) might extrapolate beyond the region where (2.3) is valid (Marquardt 1963). In such cases it will be beneficial to adjust \( p \) by only a fraction of the upgrade vector. This can be accomplished by adjusting the parameter upgrade vector by \( 0 < \mu \leq 1 \) leading to \( p_{i+1} = p_i + \mu \Delta p \), which will minimize the risk of divergence due to overshooting. Several methods can be applied to determine \( \mu \), e.g. Cooley and Naff (1990, p. 72), or the method incorporated into PEST (Doherty 2010).
\[
\mu = \frac{\sum_{j=1}^{k} r_j \omega_{jj} y_j}{\sum_{j=1}^{k} \omega_{jj} y_j}
\]

where \( y_j \) is the \( j \)’th element of

\[
y_j = X_j \Delta p
\]

and \( X_j \) is the row vector of \( X \) corresponding to the \( j \)’th observation.

2.1.2 Scaling

When including multiple types of observation data and parameters of different magnitudes, it often occurs that the individual elements of \( X \) varies by several orders of magnitude. Potentially this leads to round off errors in the calculation of the parameter upgrade vector (Cooley and Naff 1990, p. 62; Doherty 2010, p. 2-10). To circumvent this problem (2.6) is scaled by

\[
C_{ll} = (X^T \omega X)_{ll}^{-1/2}
\]

where \( C_{ll} \) is a diagonal matrix. Multiplying both sides of (2.6) by \( C \) gives the equivalent

\[
C_{ll}^{-1} \Delta p_i = (Q_i^T \omega Q_i)^{-1} Q_i^T \omega r
\]

\[
Q_i = X_i C_i
\]

Due to the scaling (2.10) is numerically far superior to (2.6) (Doherty 2010, p. 2-10). Determining the parameter upgrade vector using (2.10) is known as the Gauss-Newton method (Cooley and Naff 1990, p. 62).

2.1.3 The Levenberg-Marquardt method

The Gauss-Newton method derived in the previous section can be highly effective despite that it does not progress directly to the minimum of the objective function. However, convergence is not guaranteed for this method. As an alternative a steepest decent method could be applied. This method simply follows the steepest decent of the objective function contour given as (Aster et al. 2005, p. 174; Doherty 2010, p. 2-9)

\[
g_i = -2X_i^T \omega r
\]

Except for models having highly correlated parameters (Doherty 2010, p. 2-8 - 2-9), applying (2.11) with the appropriate damping guarantees convergence but at a slow rate (Aster et al. 2005, p. 176).

To combine the benefits of the two methods Marquardt (1963) and Levenberg (1944) derived a solution which introduces a term into (2.10) which can change the orientation of \( \Delta p_i \) in the direction of \( g_i \):

\[
C_i^{-1} \Delta p_i = (Q_i^T \omega Q_i + \lambda I)^{-1} Q_i^T \omega r
\]

It is seen directly that for \( \lambda = 0 \) (2.12) reduces to 2.10, but for values larger than zero the direction of the parameter upgrade vector is changed in the direction of \( g \) (Cooley and Naff 1990, p. 63). By recomputing \( \lambda \) and the damping parameter \( \mu \) for each iteration and by solving (2.12) instead of (2.10) the Marquard-Levenberg method becomes a more efficient and robust minimization method than the Gauss-
2.1.4 Data weighting and model errors

The weighting introduced into (2.12) balances the contribution of each observation in the inversion problem. Weighting should ideally be equal to the inverse of the variance-covariance of the true (but unknown) errors (Hill 1998, Appendix C). They can therefore only be estimated based on knowledge of the system analyzed. For head data Nilsson et al. (2006) gives an example of typical contributions to the error estimate which should be included. These are a combination of the fact that the model is unable to represent the true system analyzed (primarily scaling issues), and that the measurement of the observation might be in error and be non-stationary. Similar was already discussed by Christensen (1997) and Christensen et al. (1998) who estimated the “total error” and thus the weights to be used for hydraulic head data in a pragmatic way. However, it is beneficial to include other contributions into the estimates of the observation weights. When using different types of data these should be scaled, to be unit-less; otherwise summing them in (2.12) would produce meaningless results (Hill 1998, p. 13-14). Moreover, the weighting might be used to emphasize or reduce the contribution of certain terms in the objective function (Cooley and Naff 1990, p. 53). This could e.g. be the case when using a distributed model and the modeler wishes to achieve a more accurate data fit in a specific subpart of the model domain. Moreover, data weights could be used to balance contributions from different datasets in a joint inversion strategy (Behroozmand et al. 2012; Herekenrath et al. 2012; Paper 3). If the datasets pertaining to the submodels in a joint inversion setup have different numbers of observations it will be beneficial to scale the weights with the inverse of the number of observations in the corresponding data set (see section 2.3.1).

2.2 Stabilizing ill-conditioned or singular inverse problems

Despite the fact that an otherwise unstable inversion problem can be stabilized through the methodologies presented in section 2.1.1 to 2.1.3 the normal matrix \((X^T \omega X)\) might still be singular or near singular (ill-conditioned). Singularity of the normal matrix will occur if the columns (or rows) of the Jacobian matrix is linear dependent or nearly linear dependent (Cooley and Naff 1990, p. 60). In practice this occurs if one or more parameters are insensitive to the information contained in the calibration dataset (one or more columns in \(X\) are nearly zero) or if parameters are correlated (two or more columns of \(X\) are nearly proportional). Ill-conditioning is more prone to occur if the model contains a high number of parameters, and singularity is guaranteed if the model has more parameters than there are observations. For the inversion method presented in the previous the theoretical maximum number of parameters that can be estimated equals the number of observations. However, this is seldom the case in practice where the number of estimated parameters must be much less.

If the Jacobian matrix is estimated with sufficient accuracy, two measures can be utilized to judge if an inversion problem may be ill-conditioned. The first measure is the composite scaled sensitivity (Hill 1992; Hill 1998) defined by

\[
ccs_i = \left[ \frac{1}{k} \sum_{j=1}^{k} \omega_{jj} \left( p_i \frac{\partial f_j(p)}{\partial p_i} \right)^2 \right]^{1/2}
\]

2.13

where \(ccs_i\) is the composite scaled sensitivity with respect to parameter \(p_i\). Composite scaled sensitivities have the benefit that they are easily calculated and intuitive to understand. The measure has been used in several studies to determine the individual importance and identifiability of specific parameters (Anderman et al. 1996; Hill et al. 1998; and others). It has been shown that parameters having a composite scaled sensitivity of two orders of magnitude less than the highest value should be excluded.
from the inversion in order to prevent the inversion problem from being ill-conditioned. However, the composite scaled sensitivity is only based on a single column of the Jacobian matrix, hence it cannot determine parameter correlations. These can instead be estimated from the variance-covariance matrix computed as (Hill 1998)

\[ \text{cov}(\mathbf{p}) = \frac{\Phi}{l-k}(X^T \omega X)^{-1} \]  

2.14

The variance-covariance is a symmetric matrix with the variance of each parameter in the main diagonal, and the covariances between parameters above and below the diagonal. Based on (2.14) the correlation coefficients can subsequently be determined as

\[ \text{corr}(p_i, p_j) = \frac{\text{cov}(p_i, p_j)}{\sqrt{\text{var}(p_i)} \cdot \sqrt{\text{var}(p_j)}} \]  

2.15

where \( \text{corr}(p_i, p_j) \) is the correlation coefficient between parameter \( i \) and \( j \). If \( i \neq j \) the correlation coefficient will have a value between -1 and 1 and if \( i = j \) the correlation coefficient will be equal to 1. Since (2.14) is symmetric, so is (2.15), and off diagonal elements having values in the vicinity of 1 or -1 indicate that estimated parameters pertaining to the respective row and column are correlated.

In combination the composite scaled sensitivities and the correlation coefficients can be used to exclude parameters from the inversion that have low sensitivity or which may be correlated (Hill and Østerby 2003). However, they are both based on the linear approximation of the Jacobian matrix which will change as the inversion progresses. The measures may therefore lead to the exclusion of parameters which might be identifiable at a later stage in the inversion process. For that reason parameter correlations and composite scaled sensitivities has to be recalculated during the inversion and the truncation of the parameters reevaluated.

In the following two alternatives to the methodology presented above will be given; namely Tikhonov Regularization and the Singular Value Decomposition of the normal matrix.

2.2.1 Tikhonov Regularization

Tikhonov regularization (Tikhonov and Arsenin 1977) constrains the inversion problem by adding extra information pertaining directly to parameters estimated. This is accomplished through a regularization objective function. This methodology is presented in the following.

By acknowledging that the elements of the data vector \( \mathbf{y} \) contains noise it is evident that several solutions might exist that minimizes the objective function below this noise level

\[ \Phi_m \leq \delta \]  

2.16

where \( \Phi_m \) is the model objective function defined by (2.2) and \( \delta \) is a target objective function determined from the estimated noise level of the observation data. It can therefore be argued that all models which fall below this objective function criterion will provide equally good representations of the observation data.

If there are many parameters to be estimated it is beneficial to introduce an extra constraint to the inversion problem in the form of a preferred state of the parameter values. Such a constraint can be formulated as a regularization objective function

\[ \Phi_r = (\mathbf{d} - \mathbf{Zp})\omega_r(\mathbf{d} - \mathbf{Zp}) \]  

2.17
where \( d \) holds the regularization observations, which could be regarded as a preferred state of the system; \( Z \) is a matrix describing the relation between the parameters and the elements of \( d \); and \( \omega_r \) holds the regularization weights. If the elements of \( Z \) are dependent on the parameter values, the regularization constraints are nonlinear and it must be linearized. This can be accomplished similarly to (2.3). Two types of regularization constraints are often used: the preferred value regularization, and the minimum variation (or smoothing) regularization. Using the first methodology the preferred parameter values would be contained in the vector \( d \) and the \( Z \) matrix would be the identity matrix. Using the second method, \( d \) would be a vector of zeros and the \( Z \) matrix would contain zeros in all the rows except for the two columns pertaining to the parameters which preferentially should be equal, the elements in \( Z \) pertaining to these parameters should be 1 and -1, respectively.

Under the constraints given on the measurement objective function the regularization problem can be formulated as a damped least square problem minimizing the combined objective function given by

\[
\Phi = \Phi_m + \mu \Phi_r \tag{2.18}
\]

where \( \mu \) is a regularization weight factor added to ensure that the constraint given by (2.16) is kept. Using the Tikhonov regularization methodology implemented in PEST the regularization weight factor is therefore recalculated at each iteration step of the inversion process.

### 2.2.2 Singular Value Decomposition (SVD)

The SVD of an arbitrary matrix \( G_{m \times n} \) is given as

\[
G_{m \times n} = U_{m \times m} \begin{bmatrix} S_{n \times n} & 0_{(m-n) \times n} \end{bmatrix} V_{n \times n}^T \tag{2.19}
\]

Where \( U_{m \times m} \) is an orthogonal matrix holding the left hand side eigenvectors spanning the data space; \( S_{n \times n} \) is a diagonal matrix holding the singular values arranged in decreasing order in the main diagonal; and \( V_{n \times n} \) is an orthogonal matrix holding the right hand side eigenvectors spanning the model space (Aster et al. 2005, p. 55; Lawson and Hanson 1995, p. 18).

When analyzing inversion problems the SVD has some interesting possibilities. Hill and Østerby (2003) compared the results obtained from the SVD of the Jacobian matrix with an analysis of the correlation coefficients and composite scaled sensitivities. By analyzing the last column vector of \( V \) they found that the parameter correlations were present between parameters pertaining to the highest values in the vector. With respect to identification of parameter correlations they concluded that SVD of \( X \) was not as dependent on the accuracy of \( X \) as the parameter correlations calculated by (2.15). The SVD results were however not as intuitive to understand as the correlation coefficients.

SVD can also be incorporated directly into the inversion process. This is done through the SVD of the normal matrix \( (X^T \omega_m X) \). The inversion process can thereby be reformulated and stability can be guaranteed through truncation of \( S \). Since the normal matrix is symmetric then \( U = V \), and its SVD gives

\[
X^T \omega_m X = VSV^T \tag{2.20}
\]

Since the normal matrix is symmetric positive semidefinite its eigenvectors are orthogonal (Tonkin and Doherty 2005) and \( V^T = V^{-1} \). Using this and (2.20), (2.6) can be rewritten to

\[
\Delta p = VS^{-1}V^T X^T \omega_m r \tag{2.21}
\]

If the Jacobian matrix is singular or ill-conditioned the smallest diagonal elements of \( S \) approach zero and these eigenvalues correspond to the eigenvectors which span the calibration null space. Since these
values are very small their inverted values will dominate the solution, and amplify any noise present (Aster et al. 2005, p. 65). It is therefore beneficial to exclude these eigenvalues from the inversion. If all the eigenvalues approaching zero are excluded (2.20) can be approximated by

\[ X^T \omega X \approx [V_p, V_o] [S_p \ 0 \ 0] [V_p, V_o]^T \Rightarrow \]

\[ X^T \omega X \approx V_p S_p V_p^T \]

where \( S_p \) are the eigenvalues which are included in the estimation of the parameter upgrade vector and \( V_p \) and \( V_o \) are the eigenvectors spanning the solution and the null space respectively. (2.22) can be used to reformulate (2.21) to

\[ \Delta p = V_p S_p^{-1} V_p^T X^T \omega_m r \]

By (2.23) the vector upgrade is only done in the direction of the dominant eigenvectors spanning the solution space. This methodology for estimating the parameter upgrade vector is called Truncated SVD or TSVD. To apply the method, the modeler only needs to determine a truncation limit hereby selecting which eigenvalues to exclude from the inversion. In PEST two criteria are evaluated and the more restrictive is applied. The first criterion is fixing the maximum number of singular values to include in the inversion process, and the second is a selection based on the ratio from the highest to the lowest singular value to include in the solution.

2.2.3 Reducing dimensionality through SVD-assisted inversion

Individually or in combination the two regularization methods presented above provide powerful methodologies to stabilize underdetermined inversion problems. However, when performing highly parameterized inversion (Hunt et al. 2007) they do not reduce the computational burden of estimating the Jacobian matrix. Tonkin and Doherty (2005) presented a method which circumvents this problem while still keeping the benefits of the methods presented above. The Hybrid Regularization Methodology or the SVD-assisted inversion defines a set of super parameters (\( p_s \)) which are actually scalars for linear combinations of base parameters determined through SVD of the base parameter normal matrix. Base parameters are here defined as the complete set of parameters pertaining to the underdetermined model. After the definition of the super parameters the inversion problem is treated as a normal nonlinear inversion, by determining the sensitivities (\( X_s \)) pertaining to the super parameters. The super parameter upgrade vector is therefore determined as

\[ \Delta p_s = (X_s \omega_m X_s)^{-1} X_s^T \omega r \]

In order to determine the elements of \( X_s \) by perturbation, perturbed super parameter values must be transformed to base parameter values pertaining to the inverted model. This transformation is done through (Christensen and Doherty 2008, appendix A)

\[ p = V_p p_s \]

Because the number of super parameters (\( p_s \)) is typically much less than the number of base parameters (\( p \)), calculation of \( X_s \) requires much fewer model simulations than calculation of \( X \). Furthermore, when calculation of \( X \) is only performed once to compute the normal matrix which is decomposed by SVD to give (2.20), then minimizing the objective function using (2.24) will run much faster than by using (2.6) to compute the parameter upgrade vector, and it will also run for under determined problems.
As with the TSVD inversion, it is important to select an appropriate truncation limit. Choosing a restrictive value will reduce the number of eigenvectors included in the solution hereby reducing the information drawn from the observation dataset. On the other hand setting a too loose criteria will lead to what is typically known as over fitting whereby noise is amplified (Moore and Doherty 2005).

The SVD-assisted inversion setup was used to reduce the computational burden of inverting the locally calibrated models presented in paper 2 of this thesis. Based on the results the methodology proved to be a strong and reliant method and it therefore provided good calibration results for the present application.

2.3 Joint inversion

The following presents the methodology from paper 3 of this thesis to introduce more calibration data into a groundwater model through joint inversion of geophysical and hydrological datasets. This methodology may potentially reduce the calibration null-space defined in (2.22). The term joint inversion has been adopted from Ferré et al. (2009) and it is used to define a setup where inversion of a groundwater model is combined with inversion of a geophysical model either directly or through a petrophysical relation. This type of inversion is also sometimes referred to as hydrogeophysical inversion.

2.3.1 Inversion using multiple data types

When performing joint inversion, the different types of observation data must be contained in the objective function, which will result in the following basic structure

\[ \Phi_{\text{comb}} = (\text{nobs}_{\text{gwm}})^{-1/2} \Phi_{\text{gwm}} + (\text{nobs}_{\text{gf}})^{-1/2} \Phi_{\text{gf}} \]  

2.26

where \( \Phi_{\text{gwm}}, \Phi_{\text{gf}}, \) and \( \Phi_{\text{comb}} \) are the objective functions related to the groundwater model, the geophysical models and the combined model, respectively. The coefficient in front of the individual objective functions balances the contributions from datasets containing different number of observations, so that the model with the largest corresponding observation dataset will not dominate the solution. \( \text{nobs}_{\text{gwm}} \) and \( \text{nobs}_{\text{gf}} \) are thus the number of observations pertaining to the groundwater model and the geophysical model, respectively. Other authors have used subjective weights to balance the terms (Christiansen et al. 2011; Herckenrath et al. 2012). Using such is similar to the encouragement made by Hill (1998); that data weights should be used to scale observations providing meaningful results when being summed to estimate the combined objective function, or to reduce contribution from less reliant sources.

Finally, by adding extra model objective function terms to (2.26) extra models and datasets can be included in the inversion.

2.3.2 Linking models in the inversion process

When performing joint inversion between hydrological and geophysical models, parameter values are typically linked through a petrophysical relation based on Archie’s Law (Archie 1942). However other relations have been proposed and a review can be found in Mazác et al. (1985) and Slater (2007). One of the primary restrictions of the joint inversion methodology lies in the petrophysical relations. These are typically empirically based and do not include all the complexity that determines hydraulic conductivity. Petrophysical relations are therefore to be considered as site-specific, and empirical prefactors need to be calibrated to fit local conditions. Despite recent advances within geophysical methods, where methods, being directly sensitive to the water content of the subsurface, such as Magnetic Resonance Sounding (MRS) (Legchenko et al. 2002; and others), have been developed, these still rely on empirical petrophysical relations to estimate hydrological parameters.
When linking models together this can be done using a brute force methodology, where parameters estimated based on the geophysical model are used directly to calculate hydraulic parameters for the groundwater model, or it can be applied through regularization constraints using (2.17). Flow charts for each of these methods are presented below. Figure 2-1 shows the flowchart for the brute force methodology. In the following this methodology will be referred to as method 1.

![Flowchart](image)

**Figure 2-1: Joint inversion of a groundwater model and a geophysical model using method 1. Multiple geophysical models can be added to this setup using the same or different petrophysical relations.**

Method 1 uses a known or assumed petrophysical relation to calculate the complete or a subset of hydrological parameters directly based on geophysical parameters. The parameters that cannot be related to the geophysical parameter are treated as traditional groundwater model parameters. The forward responses for each of the models are used to calculate the objective function given by (2.26). In the inversion applying method 1 the Jacobian matrix will have the following form

\[
X = \begin{bmatrix}
\frac{\partial f_{gwm}}{\partial P_{gwm}} & \frac{\partial f_{gwm}}{\partial P_{gwm+gfm}} & 0 \\
0 & \frac{\partial f_{gfm}}{\partial P_{gwm+gfm}} & \frac{\partial f_{gfm}}{\partial P_{gfm}} \\
(regul.) & (regul.) & (regul.)
\end{bmatrix}
\]

here \( \frac{\partial f_{gwm}}{\partial P_{gwm}} \) is the sensitivity of the groundwater model observations to changes in parameters that only pertain to the groundwater model; \( \frac{\partial f_{gwm}}{\partial P_{gwm+gfm}} \) and \( \frac{\partial f_{gfm}}{\partial P_{gwm+gfm}} \) are sensitivities to the groundwater model observations and the geophysical model observations to parameters which are a part of the petrophysical relation; \( \frac{\partial f_{gfm}}{\partial P_{gfm}} \) are sensitivities of geophysical observations to changes in the geophysical parameters which are not a part of the petrophysical relation; finally, \((regul.)\) are potential regularization constraints added to the inversion, these are not mandatory. Since calculating the Jacobian matrix normally is the most time consuming part of the inversion, considerable runtime can be saved through reducing the number of model calculations. When performing joint inversion some elements of the Jacobian might hold null values. This is for instance the case in the second row in the first column of (2.27), since parameters pertaining only to the groundwater model have no relation to geophysical parameters. Similar
accounts for the first row in the third column, where only the geophysical model needs to be run. Therefore, when computing different parts of the Jacobian matrix considerable model runtime can be saved by avoiding unnecessary model calls.

Figure 2-2: Joint inversion using of a groundwater model and a geophysical model method 2. Multiple geophysical models can be added to this setup using the same or different petrophysical relations.

Figure 2-2 shows a flow chart of the joint inversion method 2. Here model parameters are not directly linked, but differences between hydrological parameters of the groundwater model and geophysical equivalents derived through petrophysical relations are minimized through a regularization objective function. Compared to method 1, parameter values derived through the petrophysical relation may therefore differ in the inversion from the corresponding groundwater model parameter values. Differences in the parameter estimates can therefore be indicative of either that the petrophysical relation is wrong or biased for the specific conditions analyzed or that the geophysical model and the groundwater model simulate incompatible systems (Similar could be concluded for method 1 results, but here it could also be indicative of structural error). The Jacobian matrix for the system presented in Figure 2-2 is given as

\[
X = \begin{bmatrix}
\frac{\partial f_{gwm}}{\partial P_{gwm}} & \left( \frac{\partial f_{gwm}}{\partial P_{gwm+gfm}} \right) & 0 \\
0 & \left( \frac{\partial f_{gfm}}{\partial P_{gwm+gfm}} \right) & \frac{\partial f_{gfm}}{\partial P_{gfm}} \\
\end{bmatrix} \quad 2.28
\]

Using method 2 parameters going into the petrophysical relation is linked through regularization constraints positioned in the bottom of the Jacobian matrix in (2.28). For that reason the two uppermost elements of the center column of (2.28) are enclosed in brackets since these no longer holds the petrophysical parameters. The parameters that are shared between the groundwater model and the geophysical model of the Jacobian matrix are therefore much fewer, and for the case presented in paper 3 they only account for layer thicknesses.
Since the regularization constraints in the present case are linear, they do not require the model to be run to estimate their derivatives, and for the sake of estimating the Jacobian matrix they do not prolong the inversion runtime. Another benefit of method 2 is that more parameters are independent (they are only linked through linear regularization constraints) which means that more models can be run independently to compute columns of the Jacobian matrix. For the cases where multiple geophysical models are linked to one groundwater model, this can result in considerable reduction in inversion runtime.

The joint inversion methodology has been developed and tested for joint inversion between MRS, TEM and aquifer test data and these results are presented in paper 3.
3 Parameterization

Parameterization of the groundwater model is presumably the most important part of the inversion process. Parameters should be defined in such a way that they through inversion can be optimized to make the model fit the available observation data as well as possible. In the following focus will be given to parameterization of hydraulic conductivity within groundwater models (the same methodologies might also be used to define other spatially varying parameters such as specific storage, porosity, etc.)

3.1 The principle of parameter parsimony

The availability of computational resources which has grown rapidly within recent years has raised questions on how models should be defined. Previously model complexity was often for practical reasons constrained by the availability of calculation resources. However, today modelers can incorporate high level of complexity into models and still be able to perform detailed sensitivity and predictive analysis. An example of this is Gallagher and Doherty (2007). Moreover, fast internet connections allows parallelized calculations to be made across networks using several computers and processors (Hunt et al. 2010). A good code example that makes this possible is BeoPEST (Schreuder 2009). The obvious question is therefore: Was the simplicity of groundwater models only used due to lack of computational resources? Or is it still meaningful to work with simple models despite that modelers might have computational resources to do otherwise? These questions can be rephrased to: Should modelers use parsimonious models or highly parameterized models? The principle of parsimony or Occam’s razor argues that models should be kept as simple as possible while accounting for the primary system processes which are important to simulate the observations and predictions (Hill 1998; Hill 2006; Hill and Tiedeman 2007). Models using this principle most often hold much fewer parameters than observations, resulting in a well-posed inversion problem, where parameters can be uniquely determined. The primary arguments for the principle of parsimony are given as (Hill 2006):

- Simple models have a high level of transparency. The modeler can hereby more easily determine the dominant processes which influence predictions and observations.
- A high level of complexity (a large number of parameters) will potentially lead to over fitting, where observation errors are fitted rather than the observations themselves.
- Simplicity often causes short runtime, making detailed sensitivity analysis more easily obtained.
- The entire complexity of the true system can never be incorporated into a model that is an inevitable simplification, also when the model is highly parameterized.

As a contrast to the principle of parameter parsimony stand the use of over parameterized models (Hunt et al. 2007). An over parameterized model often holds more parameters than observations, e.g. Tonkin and Doherty (2005) which leads to an ill posed inversion problem. These models therefore require regularization in order to stabilize the estimation problem. Arguments for utilizing over parameterized models are often

- Using TSVD the set of adjustable parameters is purely defined from the calibration dataset, and the entire content of information can therefore be drawn from the observations (Tonkin and Doherty 2005).
- Structural noise decreases with increasing parameterization, when using parsimonious models the structural noise might dominate over observation noise (Doherty and Welter 2010)
- Fixing insensitive and correlated parameters might lead to hardwired errors in the model structure (Hunt et al. 2007)
- Fixing parameters or a parsimonious structure might lead to limitations in the sensitivity analysis, since the model is not allowed to fully analyze variations and alternatives (Hunt et al. 2007)
The principle of parsimony can be thought of as a user specified form of regularization (Hunt et al. 2007).

The discussion given here is not meant to end up with an argument for either of the methods, but more as a general discussion on costs and benefits of each of them. The discussion will mainly be based on literature reviews and the results presented in paper 2.

The proponents of the two methods often have similar arguments for choosing their preferred parameterization, namely that a highly complex setup does not guarantee accurate simulations and neither does simplicity, the best model should instead be found at the middle ground (Hill 2006; Hunt et al. 2007). Moreover, they agree that even the most complex models cannot encompass the complexity of the true system. The next question is how much complexity should be included? Hill (2006) argue that initially models should be made as simple as possible, and complexity should be added slowly, and only to the extent that it improves fit to observations (within the errors) or result in more accurate predictions. Moore and Doherty (2005) on the other hand uses an over parameterized model, constrained with regularization, to determine the setup which minimizes the predictive error variance. In paper 2 of this thesis, an over parameterized model setup has been used to describe the geological complexity of the internal structure of a buried valley structure. Dimensionality has been reduced through the use of SVD, SVD-assist and Tikhonov regularization. Initially this model was defined using a parsimonious approach, however; the system could not be simulated accurately using this setup. Therefore the parameterization was redefined using pilot points, to incorporate complexity into the primary aquifers in the model.

3.2 Parameterization using zones

A very widely used methodology of parameterization of spatial varying parameters is using zones of piecewise parameter consistency (Christensen 1997; Christensen et al. 1998; Henriksen et al. 2003; Jeppesen et al. 2011; Jørgensen et al. 2008; Kim et al. 1999; and others). The methodology is intuitive and easy to implement, since the parameter values apply directly to each cell contained by a specific zone of the groundwater model. The delineation of zones is often defined based on a thorough geological, hydrological, and/or geophysical analysis. However, determining specific locations of boundaries can be difficult, especially in parts of the model domain where the data density is small. Moreover, using this parameterization methodology means the internal heterogeneity within the zones cannot be represented. This can potentially lead to introduction of new zones in the model that are not based on the geological model but serves merely as a device for achieving better correspondence with observations (e.g. Kristensen 2003). However, in many groundwater modeling contexts sharp interfaces between different geological units must be represented. This can for example be the case when setting up models describing buried valley structures incised into a low permeable substratum, when dealing with faults, or more generally when going from one geological setting to another. For these purposes use of zones is an obvious choice.

3.3 Parameterization using pilot points

As a contrast to the sharp boundaries represented by zones stands the use of pilot points for parameterization. Using this method means that the model parameter values are estimated at the pilot points that are scattered throughout the model domain. Based on their values a corresponding model parameter field is generated using interpolation from the pilot points to the groundwater model cells. This field is used in the groundwater model when making simulations. The pilot point methods has been used for several years (Certes and De Marsily 1991; LaVenue and Pickens 1992), and it has grown particular popular within recent years in connection with over parameterized models (Alcolea et al. 2008; Christensen and Doherty 2008; Fienen et al. 2009; Herckenrath et al. 2011). The optimal location and number of pilot points has been subject to a number of studies (LaVenue and de Marsily 2001; Mehne
2011), however the most often used method used is still either liberally placement with increased point density in heterogeneous areas (Doherty 2003), or a regular grid of points.

An important part of the parameterization using pilot points is the methodology of interpolation. Depending on the number of pilot points used in the analysis, the choice of interpolation methodology will have more or less influence on the estimated field. A widely used interpolation method is kriging. The theory of kriging can be found in several textbooks including Kitanidis (1997); Webster and Oliver (2007); and others. Kriging is a smooth interpolator, which often produce hydraulic conductivity fields that appear realistic. Moreover, the kriging interpolation weights can be computed solely from the spatial distribution of the pilot points; these weights can therefore be estimated once prior to commencing model inversion. Using kriging, the spatial interpolation is normally based on the covariance or the semivariance of the measured variables. The variogram describing the variation of hydraulic conductivity should therefore be estimated based on the expected variation within the hydraulic conductivity field. Since hydraulic conductivities can potentially vary over several orders of magnitude, it is good practice to interpolate fields working in the logarithmic space, and then transforming fields back to their natural values prior to commencing a model run (Certes and De Marsily 1991).

3.4 Combining pilot points with zones

Pilot points in combination with zones can prove to be an effective parameterization methodology. Zones can define sharp boundaries between different geological units, while pilot points can be used to model heterogeneity within these zones.

Figure 3-1: Example of a hydraulic conductivity field created by a combination of pilot points and zones of piecewise constant values. In the hatched area, parameter values are defined through zones. This area comprises primarily low permeable clays which the buried valleys (the un-hatched area) are incised into, and some sand units. In the unhatched area variation in hydraulic conductivity is defined through pilot points. Here a smooth variation is seen, which is meant to describe a diluvial environment.

Figure 3-1 shows an example from paper 2 where zones have been used in combination with pilot points. The figure shows the hydraulic conductivity field of a buried valley structure incised into a low permeable substratum. It is apparent that the use of pilot points in this example introduces an internal heterogeneity in the buried valley which had been impossible to shape using zones. However, the sharp boundary between the valley and the low permeable deposits would have been similarly difficult to make using only pilot points. Some parts of the buried valley show patterns which resemble those defined
through zones. This is because the particular hydraulic conductivity field shown in Figure 3-1 in these parts is generated from averaged values from a geological model (see section 3.5).

3.5 Applying an upcaled geological model to the numerical model

Modellers are often faced with the problem of geological variation at a scale smaller than represented by the numerical resolution of the groundwater model. Under such conditions these variations must either be ignored or incorporated in the model. Upscaling heterogeneity in hydrological studies has been the topic of a large body of research, and a review is given by Sanchez-Vila et al. (2006). In the present thesis the method known as Power Averaging (Fleckenstein and Fogg 2008; Sanchez-Vila et al. 2006) has been employed to calculate effective hydraulic conductivities over a block. For the present studies (namely paper 2) this method gives accurate results, it is simple to implement, and it provides fast upscaling making it easy to use in connection with inverse methods.

A schematic description of the method is presented in Figure 3-2. The black lines on the cross section indicate elevation of the numerical layers in the groundwater model. In between these layers the hydraulic conductivity pertaining to the geological model voxels are averaged using a weighted mean to estimate an effective hydraulic conductivity for the pertaining cell in the groundwater model. The horizontal scale of the geological and the numerical model are equal. It is therefore avoided to make horizontal interpolation within the groundwater model cells, which is difficult to do in a meaningful way.

![Schematic description of a voxel based geological model (left) and the principle of the upscaling methodology (right) used for creating input to the numerical groundwater model.](image)

The effective horizontal hydraulic conductivity is estimated as the weighted arithmetic mean of the geological units given as

\[
K_h = \frac{\sum_{i=1}^{n} z_{GeoLn} K_{GeoLn}}{\sum_{i=1}^{n} z_{GeoLn}}
\]

where \(z_{GeoLn}\) denotes the thickness of the part of the geological model voxel located within the numerical layer, and \(K_{GeoLn}\) denotes the hydraulic conductivity of that voxel. This methodology can also be used for calculating for example the effective specific storage values to be used in the groundwater model.

Similarly, the effective vertical hydraulic conductivity can be calculated as the weighted harmonic mean of the hydraulic conductivities of the geological model voxels using
Applying this methodology in MODFLOW is easy since the effective hydraulic conductivities can be written directly to the lpf package (Harbaugh et al. 2000) input file. However, it has one apparent drawback. Effective hydraulic conductivities are calculated over a larger block than the one used for calculating the conductance terms given in (1.5). Conductances will therefore be influenced by geological units which are not located in between the groundwater model nodes (see right hand side of Figure 3-2). This can potentially lead to biased horizontal and vertical hydraulic conductances, and the influence of such should always be investigated when applying the method.

\[ K_v = \frac{\sum_{i=1}^{n} Z_{GeoL_i}}{\sum_{i=1}^{n} K_{GeoL_i}} \]
Burried Quartenary valleys and their importance for groundwater groundwater resources

In large parts of the world, the geological structure near terrain is dominated by glacial activity, which has lead to the formation of buried valleys. This is for example the case in the northern part of Western Europe (Huuse and Lykke-Andersen 2000), the United States of America (Kehew and Boettger 1986; Ó Cofaigh 1996; Ritzi et al. 1994), and Canada (Desbarats et al. 2001; Ó Cofaigh 1996; Russel et al. 2004). Buried valleys often contain important groundwater resources used for irrigation, industrial and drinking water purposes. In the following their origin and structure will be briefly described as will methods for their mapping. Their influence on groundwater flow and how this can be modeled will also be explained.

4.1 Structure and origin

Buried valleys are often found as large elongated structures cut into unconsolidated sediments or bedrock (Ó Cofaigh 1996). They can occur as either being completely or partly buried, where the latter has a present day counterpart which can be observed in terrain (Sanderson and Jorgensen 2003). Several theories have been presented on the origin of these structures, and a review and evaluation of these can be found in Huuse and Lykke-Andersen (2000). They compile the dominant theories into the following categories: steady-state sub-glacial drainage of meltwater and groundwater driven by hydrostatic pressure gradients, catastrophic meltwater discharge (jökulhlaups), glacial erosion, erosion by rivers during glacioeustatic lowstand, aggradation (stacking) of delta channels, and tidal scour. They conclude that the dominant factors can be narrowed down to the first three, which all are related to activities of former ice sheets. Moreover, they conclude that the valleys presumably have a polygeneric origin given as a combination of these processes.

Buried valleys have several characteristics, including highly irregular undulating floors, they sometime terminate abruptly (Jorgensen and Sanderson 2006), and they often have thresholds located either perpendicular or parallel to the valley orientation (Kehew and Boettger 1986; Shaver and Pusco 1992). Moreover, they often have a very complex internal structure. Gravesen (1994; 1996; 1997) made a detailed analysis of a buried valley structure, and mapped deposits including till units, melt-water sand and gravel, fluvial sand and lacustrine clay and sand.

Comprehensive statistical analysis by Andersen et al. (2012) shows that the Danish buried valleys are 500 m to 1500 m, 50 m to 200 m deep, and are equally likely to be U-shaped, V, shaped or flat-bottomed. The slope of the valley flanks can be up to 45° or more (Jorgensen and Sanderson 2006), but even steeper gradients have been observed for valleys incised into bedrock (Sharpe et al. 2002). Andersen et al. (2012; Jorgensen and Sanderson 2008); and Russel et al. (2004) found that buried valleys often have been reused during successive glaciations leaving the valleys with multiple cut and fill structures or channels, and that tectons caused by glacial activities could have disturbed the infill as well. Such cut and fill structures are also weekly indicated by a seismic survey in the Ristrup-Grundfor-Ødem valley (Blæsbjerg 2006) which is the field site studied in paper 2.

4.2 Mapping

The extent and shape of buried valleys can most effectively be mapped using non invasive geophysical methods. Boreholes on the other hand provide valuable information to determine the age and type of the infill deposits (Krohn et al. 2009), but they are rarely sufficiently densely spaced to be used in the mapping (Thomsen et al. 2004). Especially the transient electromagnetic (TEM) method has proven effective for locating buried valleys (Auken et al. 2008; Auken et al. 2003; Danielsen et al. 2003), and it has been used extensively for the mapping of these structures in Denmark (Jorgensen and Sanderson 2009a) and in
Germany (Rumpel et al. 2009). The TEM method can only be used in areas exhibiting resistivity contrasts between valley infill and the surroundings. Preferentially the valleys should be incised into low resistivity deposits with infill comprising dry or freshwater saturated sand or gravel (Jørgensen et al. 2003b). The resolution can however be improved using an effective inversion methodology and prior information from boreholes (Auken et al. 2008). TEM surveys are often combined with the use of reflection seismics (Jørgensen et al. 2003a; Jørgensen and Sandersen 2009a) which can provide detailed information on the internal structure of the valleys. However due to the high cost of collecting seismic data, this method is often only used at carefully selected locations. Based on the cost of the individual methods Jørgensen et al. (2003a) suggested that mapping of buried valley structures should be performed in the following steps: First, the regional resistivity structure should be determined using the TEM method. Second, seismic investigations should be used to determine the structure of the buried valleys and their surroundings, and finally should the boreholes be used to provide lithological and stratigraphical information.

4.3 Importance for groundwater flow

Because of increasing stress on near surface aquifers caused mainly by contamination and overexploitation (Huuse et al. 2003; Sandersen and Jørgensen 2003) focus has been given to deep aquifers located in buried valleys. However, buried valleys can influence the availability of groundwater resources in several ways. Based on numerical studies Seifert et al. (2007) showed that buried valleys which cut through existing geological layers can create pathways for rapid spreading of pollutants from the surface. Moreover, they showed that this could not be derived from the hydrological data alone, because their numerical model also could be accurately calibrated to the observation data using a model which did not contain the buried valley structure. Based on the results they advocate the use of a sound conceptual model for the description of the buried valley structure. Similar results were obtained by Harrar et al. (2003) for another area containing a buried valley. They showed that different models could calibrate the same dataset, hereby advocating the use of different conceptual models, but constraining them with prior information on the geological structure. Through numerical modeling Smerdon et al. (2005) showed how buried valley aquifers can influence flow in a regional scale groundwater system through seepage from overlying reservoirs, and advocated the use of numerical models for describing such systems. In combination the cited references demonstrate the importance of having specific knowledge of the shape and location of buried valleys and it shows why numerical models can be a strong tool for the assessment of the risks of influencing and contaminating the groundwater resources.

4.4 Mapping of buried valleys in the Aarhus Nord Area

The field site investigated in paper 2 is located in an area with multiple buried valley structures (see Figure 4-1). These are primarily incised into Paleogene clay deposits and the infill primarily comprises diluvial sand and gravel at most locations. However, units of till, and lacustrine sand and clay are found as well (e.g. Gravesen 1997). These structures can therefore be mapped effectively using the TEM method. Several campaigns have mapped these structures using the conventional TEM method, PATEM (Sørensen et al. 2000) and the airborne SkyTEM (Sørensen and Auken 2004) systems. Some areas have been densely mapped using especially PATEM and to a less degree SkyTEM, where others have been less densely sampled using the conventional TEM method. This accounts for the area near Ristrup well field which is the primary focus area in paper 2. The TEM soundings in this area are scattered and only of sufficient quality to provide reliable information of the bottom of the buried valley, but they provide little information on the infill of the valley structure. In the initial part of this Ph.D. project the intention was to use the TEM soundings located around Ristrup well field to constrain the pilot point values for the model presented in paper 2. However, due to the insufficient information about the internal valley structure contained in the dataset, this part of the analysis was abandoned. The joint use of geophysical and hydrological data was instead tested using the joint inversion between MRS, TEM and aquifer test
data presented in paper 3. This joint inversion methodology should still be pursued due to the great density and availability of TEM soundings in Denmark; however, this is left for future scientific work.

Figure 4-1: Description of data coverage and buried valleys located in the Aarhus Nord area which is the primary focus area of this thesis, and the area analyzed in paper 2. The buried valley structures shown on the figure are based on the descriptions of Jørgensen and Sandersen (2009b).
5 Résumé, paper 1: Evaluation of MODFLOW-LGR in Connection with a Synthetic Regional-Scale Model

5.1 Introduction

This paper tests and compares what can be gained using two grid refinement methods, namely the shared node (SN) (Mehl and Hill 2004; Mehl and Hill 2005) and the Ghost-Node (GN) method (Dickinson et al. 2007) to incorporate geological complexity in a groundwater model. When applying local grid refinement (LGR) a locally refined model (the child model) is coupled to a regional scale model (the parent model) having a coarser numerical resolution. The parent model determines the outer boundary conditions for the child model, and when using an iterative coupling, the child model determines internal boundary conditions for the parent model. This study compares the SN-LGR and the GN-LGR methods with a globally refined (GR) model having a fine grid covering the entire domain and a globally coarse (GC) model with a coarse grid everywhere. The comparison tests the methodologies used to correct for interface effects between the child and the parent model using the SN method; it tests the importance for resolving the geological resolution compared to resolving the numerical resolution; and it tests how sensitive the solution is to the stop criteria chosen for the LGR solutions.

5.2 Model setup and results

The study uses the synthetic geological models presented in Figure 5-1 and Figure 5-2 which were inspired by the geological setting at the Ristrup well field site studied in paper 2. Figure 5-1 shows the elevation of the terrain model and the top elevation of the deposits which the buried valley is incised into. Figure 5-2 shows a cross section through the locally refined area marked with a square on Figure 5-1. The figure shows the geological resolution used in two different LGR setups, one having a high geological resolution (LGR-R) and one having a coarse geological resolution (LGR-C), which is the same resolution as that used in the parent model.

Figure 5-1: Schematic description of the terrain and the bottom of the buried valley (top of the green cells in Figure 5-2). The square shows the locally refined area. The cross sections shown on Figure 5-2 only cover this area.

Figure 5-2: Cross sections showing the differences in geological resolution used for comparing the importance for the geological resolution of the model.
Figure 5-3 shows results obtained by comparing the GC model and the two LGR models, LGR-C and LGR-R. The errors shown in the figure were calculated by subtraction of simulation results obtained by the GR model; the errors are absolute values averaged over the model domain.

The results clearly show that there is a gain in accuracy using a model with a locally refined grid. Both heads and flows are more accurately simulated by using the LGR models. Increasing the geological resolution does not affect the number of parent-child model iterations nor the model runtime, and it does also not seem to have a major influence on the simulation accuracy. For the field test modeling in paper 2 of this thesis it was also found that increasing the numerical resolution around a buried valley gave larger accuracy gain than subsequently increasing the geological resolution in the model.

Further insight into the importance of geological resolution can be seen from Figure 5-4. The figure shows a contour plot of the head errors for a horizontal cross section through the two LGR models shown on Figure 5-2. It is apparent from the plots that large errors are introduced locally around heterogeneities (valley flanks) if the coarse geological model is applied. It will be critical if this model is used for making predictions that are sensitive to such geological discrepancies.

As it is apparent from Figure 5-3 the runtime of the reference model (GR) is shorter than the runtime of the LGR models. This shows that it is not always beneficial to apply a locally refined model instead of a globally refined model, because the iterative coupling of LGR can be time consuming. This accounts for both the SN method and the GN method.

Further analysis have shown, that for the present problem, the child model should only comprise up to app. 15% of the refined model area for the LGR models to run faster than the GR model. This ratio is likely to be problem dependent.

Results have shown that LGR runtimes depend on the variation of hydraulic conductivity within the individual parts of the model. Model runtimes increased for increasing hydraulic conductivity contrasts. This accounts for both the reference model and the LGR model, but the dependence was largest for the LGR models.

Figure 5-4: Errors in heads in a horizontal cross section through the LGR models. The black lines indicate the edges of the valley structure. It is evident that locally around heterogeneities large errors are introduced using a flawed geological resolution.
5.3 Conclusions

This paper provides a thorough test and analysis for the application of the iterative LGR methods of MODFLOW to simulate groundwater flow in an area with large hydraulic conductivity contrasts (a buried valley incised into a semi-permeable deposit). It is shown how MODFLOW-LGR can be used to increase both the numerical and geological resolution of a regional scale groundwater model in order to achieve more accurate simulation results. Comparing the SN and the GN methods of MODFLOW-LGR did not suggest one method to be superior to the other. For practical purposes, the GN method is simpler to set up because it does not require compensation for parent/child interface effects. However, making such corrections can easily be automated thus make the SN method just as attractive to use. Deciding if and how to apply the LGR method should rely on several considerations: does a regional scale model exist that can be used as a parent model; what is the accuracy needed at the shared interface boundaries (should the coupling be iterative or one-way); and how large a portion of the domain is of primary interest. If a regional scale model already exists, this model can be used as a parent, whereby the tedious work of constructing a model covering a sufficiently large area to achieve well defined boundary conditions can be avoided. If interface boundary conditions are expected to have little influence on model simulations and predictions, a one-way coupling might be sufficient to achieve accurate results. This might, however, be difficult to judge prior to actually running the model (Mehl et al. 2006). Finally, if only a small portion of a regional scale model is of interest, the LGR methods are model runtime competitive compared to a globally refined model and LGR can easily be used to increase numerical as well as geological resolution locally.
6 Résumé, paper 2: Influence of numerical discretization and geological resolution on groundwater model predictions of impact of a new well field – calibration and post-audit

6.1 Introduction

This paper builds on the experiences drawn from paper 1 to utilize MODFLOW-LGR to increase the numerical and geological resolution of a regional-scale groundwater model to improve local-scale predictions. Moreover, it investigates the prediction capabilities of models calibrated using different datasets by comparing simulations made by the calibrated models to observations made during an eight-year period including the first years of pumping from a newly established well field. The individual flow models are based on a separately defined geological model having a finer vertical resolution than the numerical flow model. Prior to running the numerical model the geological model is upscaled to generate input files for the numerical models (see chapter 3.5). Models are calibrated using the methods presented in chapter 2.2 using a parameterization that combines pilot points and zones and which is described in chapter 3.4. The study compares the three following basic model setups that cover the area outlined in Figure 6-1.

- A regional model setup using a numerical grid scale of 500m × 500m. This model is named GC.
- A locally refined (LGR) model using the GC model as a parent model. The LGR model has a numerical resolution of 100m × 100m but a geological resolution equivalent to the GC model. This model is named LGR-CG.
- A LGR model for which the numerical grid is identical to the former, but for which the geological resolution is also refined around the buried valley structures in the area. This model is named LGR-RG.

Figure 6-1: The field site used in the analysis, showing the location of the regional scale model and the locally refined models.

The three models presented above were each been calibrated to four datasets, these being:
• Head data covering the period 1996-2001 from the locations shown in Figure 6-1 (marked with green triangles). Models calibrated to this dataset are only named after the models presented above.

• The same dataset as presented in the previous bullet combined with drawdown data from an local aquifer test conducted near the Ristrup Well Field. Models calibrated to this dataset are called “model-name-pt”

• Head data covering the period 1996-2001 but only from within the locally refined area shown in Figure 6-1. Models calibrated to this dataset are called “model-name-local”

• The same dataset as presented in the previous bullet combined with the aquifer test data. These models are named “model-name-pt local”

6.2 Results

Typical calibration results for selected boreholes are shown in Figure 6-2 for the time series data and in Figure 6-3 for the aquifer test drawdown data.

By comparing the left (regionally calibrated models) with the right (locally calibrated models) in Figure 6-2 it is evident, that the locally calibrated models fit data more accurately. Moreover, it is clear that inclusion of the aquifer test dataset increases the simulated fluctuations between summer and winter months. By comparing results obtained with the two LGR models (LGR-RG and LGR-GC) it is evident
that these models fit the calibration data equally well and much better than the GC model having a coarse numerical resolution. This is in good accordance with the findings presented in Paper 1, where it was concluded that the numerical resolution apparently has more influence on simulation accuracy than the geological resolution.

Figure 6-3 presents drawdown simulations with the models calibrated to the aquifer test dataset. The models having a coarse numerical resolution are not capable of fitting the observed drawdown. This is expected, since this model has a horizontal cell size of 500m × 500m which is too coarse to accurately represent drawdown in the vicinity of an abstraction well located in a 1000m wide buried valley. Despite that one of the LGR models also has difficulties fitting the aquifer test data it is again observed that when calibrating to local data the numerical resolution is more important than the geological resolution.

Examples of results from the validation (or test) period, including the first years of pumping from the new well field, can be seen in Figure 6-4. Some of the characteristics seen for the calibration period are recalled for the validation period. First, dynamics of the models calibrated to the aquifer test dataset are higher than for the models calibrated only to time series data. This is especially evident for the LGR-RG-pt and the LGR-CG-pt calibrations. Moreover, the GC models generally perform poorly for the validation period; their predictions are biased. The best performing model is the LGR-RG local model which was calibrated only to fit the local time series data. It performs somewhat better than the LGR-CG local calibration despite that their fit to calibration data are similar.
The exaggerated fluctuations seen for the models calibrated to the aquifer test dataset are caused by underestimated storage parameters. However, drawdown responses shown on Figure 6-4 are also generally exaggerated by these models and to an extend which cannot be explained by low storage parameters. By comparing the right and the left plots of Figure 6-5, it is observed that the calibration including the aquifer test data results in a more closed system. The model calibrated to the aquifer test has lower hydraulic conductivity for both the deposits surrounding the valley structure and the hydraulic barrier cutting the valley into two segments in the top right of the figure. Regarding the valley infill, some resemblance can be seen between the two calibrations. Both seem to have a higher hydraulic conductivity towards the south-east of the valley structure and a low hydraulic contact through the valley structure towards the south-west. Also, on the smaller scale, differences can be observed between the two hydraulic conductivity fields. These results are judged to indicate insufficient model parameterization or, more seriously, model error.
6.3 Conclusions and perspectives

This paper tests the importance of numerical and geological resolution of a groundwater model when making prediction of local scale water resource problems. The models cover a geologically complex field area where a new well field has been established which draws groundwater from a buried valley. Especially increasing the resolution of the numerical model did improve the calibration capabilities of the groundwater model. The resolution of the geological structure in the model also proved to be important by making model predictions more accurate when compared to field observations from the validation period. Both the model having a coarse geological resolution as well as the model having a refined geological resolution could be calibrated to the observation data, but when analyzing model prediction capabilities the model with the refined geology turns out to be superior.

Models were calibrated to either time series of heads or both to time series and aquifer test data. The latter calibrated models were found to have a reduced prediction capability due to underestimated hydraulic conductivities and specific storage parameters. Despite that the aquifer test provided important information in the initial phase of the study, it did not improve the numerical model when used for calibration and prediction. This is likely to be caused by the model setup used in this study. Studies of Mishra and Neuman (2010); Mishra and Neuman (2011); Moench (2008); Nyholm et al. (2002); Poulsen et al. (2011) shows that when analyzing aquifer test data from an unconfined aquifer by using a model that assumes instantaneous release of water can lead to too small specific yield estimates. Such a model have been used in the present study, this is therefore likely to explain the underestimated storage parameters.

Depending on the calibration dataset applied, small but important differences occurred in the calibrated hydraulic conductivity fields. This can be explained by equivalences, namely that multiple hydraulic conductivity fields are capable of calibrating the analyzed datasets. This problem could be a topic for further scientific work. It is expected that inclusion of geophysical data could help constrain the inversion problem hereby resulting in a more uniquely determined hydraulic conductivity field. This could be done through joint inversion where geophysical models are inverted together with the numerical groundwater model using regularized constraints between the two. The methodology is described and tested in paper 3 using a two dimensional numerical groundwater model, an MRS model and a TEM model. The utilization in a three dimensional environment does however require further development and testing.
7 Résumé, paper 3: Joint inversion of aquifer test, MRS and TEM data

7.1 Introduction

This paper documents a novel methodology for fully joint inversion between models simulating Magnetic Resonance Sounding (MRS), TEM and aquifer test data. The methodology is tested on a synthetic dataset comprising a two aquifer system separated by an aquitard. The paper tests two different inversion methods. The first (method 1) uses a brute force coupling, and the second (method 2) uses a softer coupling based on regularized constraints between parameters estimated from the geophysics and parameters of the groundwater model. Both inversion methods were briefly described in chapter 2.3.2. The methodologies are based on an empirical relation between water content and decay time estimated using MRS and hydraulic conductivity. The TEM dataset is used to constrain the MRS inversion as well as to provide information about layer thicknesses. Testing the joint inversion schemes shows that accurate estimates of hydraulic parameters, geophysical parameters, layer thicknesses and parameters pertaining to the empirical relation can be obtained. Moreover, by joint inversion of the entire dataset parameter uncertainties can more easily be quantified than if the inversions are made separately.

7.2 Result examples

An example of the inversion results can be seen from Figure 7-1. The dataset inverted originates from a synthetically generated model contaminated with noise in order to mimic field conditions. In order to get the full benefit of the geophysical methods, layer thicknesses were allowed to vary throughout the inversion process. To implement this in the groundwater model the numerical discretization of layers had to be updated at each iteration step to conform with the estimated thicknesses. From Figure 7-1 it is apparent that good agreement can be obtained between estimated and true parameter values. Moreover, the empirical prefactor linking the geophysical model and the groundwater model can be estimated simultaneously. For the analyzed problem one inversion method cannot be judged to be superior to the other. Both methods result in good agreement with the true model structure, layer thicknesses, and parameter values.

Figure 7-1: Estimated parameter values using the joint inversion methodology
7.3 Conclusions and perspectives

Paper 3 describes two effective methods for joint inversion between a numerical groundwater flow model, and MRS and TEM models. The methods have been tested for a synthetically system and was found to work well. They still have to be tested on a field case; however, finding such a case with data of sufficient quality was much more difficult than anticipated. In the final stage of this Ph.D. project such a dataset was identified in the United States. This is currently being analyzed, but results are not ready for presentation at the time of writing.

The joint inversion methodology is very promising. MRS is a unique geophysical method in the sense that it measures directly on water content and the pore structure of the subsurface, thereby making it more directly related to hydraulic parameters than other more commercially used geophysical methods. During this Ph.D. study the joint hydrogeophysical inversion has also been tested for other synthetic model setups. One of these is a smooth or many-layer inversion of the geophysical data coupled to the groundwater model through interpolated values. This setup is schematically explained in Figure 7-2. Coupling between the groundwater model and the geophysical model is based on values interpolated between layers. This sort of setup could be beneficial for resolving heterogeneities within an aquifer that can hardly be monitored by an aquifer test but where MRS can resolve vertical variation in parameters related to hydraulic conductivity. MRS also has the potential to provide information on storage parameters in a specific aquifer (Lubczynski and Roy 2007), but to establish an approximate relation requires further research.

Tests have also been conducted on applying MRS in a three-dimensional model context. The potential for such an application is massive. It could for example be used for constraining pilot points resulting in a more uniquely determined hydraulic conductivity field for the case presented in Paper 2. However, more experiences must be drawn from the presented two-dimensional case before proceeding to a three-dimensional application.

Figure 7-2: Methodology for coupling aquifer test data with MRS data using a smooth/many layer model
8 Conclusions and perspectives

This thesis investigates methods for incorporating geological complexity into numerical groundwater models. This has been done using a combination of local grid refinement, up-scaled geological models, pilot point parameterization and joint hydrogeophysical inversion. It is documented that the MODFLOW-LGR method provides an effective method for downscaling regional scale groundwater models. However, when applying the iterative coupling model runtimes can become long and potentially lead to lack of convergence especially for models having a high coefficient matrix condition number. Under such conditions, the locally refined part of the model domain must constitute only a small portion of the regional scale model, or it should only use a one-way coupling; otherwise it may be computational more efficient to use a fine discretization of the entire region. Combining results from a synthetic test model and a field test model employing the MODFLOW-LGR method it is demonstrated that the numerical resolution of a groundwater model often has a larger impact on model simulation accuracy and calibration than the geological resolution. This was determined by calibrating and comparing the fits of models having different numerical and geological resolutions. However, for the field test the geological resolution was found to be more important when utilizing calibrated models for prediction purposes. Here predictions made with models having the more accurate geological resolution were in better agreement with the data from the validation period. When using calibrated models for prediction these should first be validated against datasets similar to prediction conditions. This is argued based on validation results covering both conditions similar to the calibration period and conditions which deviate from these (the initial phase of a well field). Results show that a subset of the calibrated models agrees well for the first part of the validation period, but they deviate considerably from the data for the period after the stress of the system changes.

The field case model was parameterized using a combination of pilot points, zones, and up-scaling of geological structures. This combination was found to be hydrogeologically sufficiently flexible and inclusive to simulate groundwater flow within and around a buried valley structure. The use of zones allowed for exact delineation of the interface between different geological structures such as the buried valleys and their surroundings. The use of pilot points allowed for description of heterogeneity internally in the valleys. And the up-scaled geological model was used to include effects from heterogeneity at a scale smaller than that of the numerical model. Determination of the internal variation in hydraulic conductivity based on pilot points proved to be influence by the dataset used for model calibration. This shows that further constraint on hydraulic conductivity variation could result in a more accurate model structure, hereby potentially improving model predictions. Such constraints could potentially be enforced through joint inversion with geophysical data.

For achieving a better understanding of applying geophysical constraints on hydrological inversion, a joint hydrogeophysical inversion methodology between MRS, TEM and aquifer test data was developed. By applying this methodology to a synthetic test case it was documented that improvements can be obtained for both the hydrological and the geophysical models, hereby achieving better understanding of the system analyzed. In the present case this can be exemplified by the joint inversion providing information on the presence the hydraulic properties of a concealed aquifer that were not reached by any of the wells or boreholes. Moreover, the methodology allows propagation of uncertainties of all datasets through the inversion process improving quantification of parameter uncertainties. By applying the regularized coupling methodology presented in this thesis it is possible to use several hydrological and geophysical models in a computational efficient way. This is done by splitting the calculation of the sensitivities contained in the Jacobian matrix on individual model calls hereby reducing the combined computational burden. Furthermore, increased efficiency can be achieved through parallelized computations. Using this methodology the perspective is to perform a full three dimensional inversion
where geophysical data is used for constraining the variation in hydraulic conductivity within the groundwater model domain.

Several of the methods documented in this thesis could be topic of further scientific work. The methodology used for geological up-scaling determines an efficient hydraulic conductivity which goes into the groundwater model. This methodology could be improved by calculating the conductance term going into the numerical model coefficient matrix directly on basis of the geological structure. Using such a methodology would remove the risk of introducing a bias into the model from geological units which are not located in-between nodes of the numerical model cells. For implementation into MODFLOW, this methodology would require a modification of the MODFLOW LPF package similar to that implemented in the HUF package.

The use of local grid refinement could be improved through a direct solution of the regional scale and the local scale groundwater flow problems. The use of the potentially time consuming iterative balancing between the local scale model and the regional scale model can hereby be avoided. Such a methodology would make MODFLOW-LGR directly comparable with finite element methods which have a more inherent grid refinement structure. However, the benefit of the MODFLOW model is that it is widely used. By implementing an unstructured grid approach would thereby make efficient local grid refinement accessible to a huge community. Such a directly coupled methodology is currently being developed by Steffen W. Mehl, USGS (pers. com.), and it will be exciting to see comparisons with the methodology used in this study.

Integrated or joint inversion between hydrological and geophysical models has great potential. The low costs of collecting geophysical data compared to hydrological data make these methods the obvious choice for constraining parameters in hydrological models. Several authors have presented methods to do so but the methods are still not being used on a routine basis. Further scientific attention should therefore be given to methods which integrate these two methods in an efficient way. The regularized joint inversion methodology documented in this thesis provides an effective tool for such application. However, further attention needs to be given to how this methodology can be applied with three dimensional groundwater flow models.
9 References:


Kristensen, M. "Indsatsområde Århus Nord 02, modellering, kalibrering (in Danish)." Hørsholm, Denmark.


McDonald, M. G., and Harbaugh, A. W. "A MODULAR THREE-DIMENSIONAL FINITE DIFFERENCE GROUND-WATER FLOW MODEL." Dallas.


Webster, R., and Oliver, M. A. (2007). *Geostatistics for Environmental Scientists*: John Wiley & Sons Ltd.

