Interfaces in coupling of hydrogeological modeling systems

Preface

The idea for this book was developed during long periods of numerical hydrogeological modeling with very interesting topics and for diverse applications. In all cases, the numerical groundwater models were not alone. They were surrounded by hydrological models for groundwater recharge, runoff modeling of small creeks and large rivers, modeling of the unsaturated zone and surface runoff, preferential flows and even climatic developments. On the other hand, there were geological models of unconsolidated and hard rocks with simple and complex structures, with anthropogenic impacts on the geology over time, for local projects and for regional areas. And for these modeling approaches – sometimes at the cutting edge of research – new questions arose: How can this modeling system be connected to this one? How should the interface be established? In most cases, a technical or practical solution was found quickly, either via a simple data transfer or via some kind of coupling. However, a systematical view on these interfaces was lacking: How do they influence the stability of the whole modeling approach? Where are these interfaces weak and where are they strong? What makes them weak or strong? How will they influence the results?

Many questions were discussed over a long period of time with a lot of colleagues, starting at the company WASY (Berlin, Germany) where I have to thank Helge Albert, Bernd Pfützner, Wolf Pagenkopf, Stefan Kaden, Ingo Michels, Andreas Krone, and especially Junfeng Luo, Katherina Fröhlich, “Bertram” Monningkoff, Ulrich Schott and Peter Schätzl. At the Free University of Berlin, some field methods that provided another perspective on hydrogeological parameters were discussed; many thanks to Asaf Pekdeger (†) and Andreas Winkler. During this time, discussions with Maria Schafmeister about geostatistical applications in numerical models were very interesting and opened new horizons. During my time at the Geological Survey of Germany, Klaus Krampe and Peter Winter were the heads of the department in which I had the chance to set up a large model that involved some interesting facets of field investigations and geological modelling, and they gave me the chance to contribute to the Hydrological Atlas of Germany. The numerical groundwater modeling does not stand alone; the consideration of environmental aspects, biological settings, landscape planning, and urban planning is essential for scientific research in some case studies in order to gain a better understanding of interdependencies. The discussions with specialists of these fields in an NGO (Friends of the Earth) were very helpful, but they also demonstrated the political consequences of scientific work in water resources planning. My work in the Advisory Board of the Berlin Waterworks was also an influential factor for this book, and I must thank Ursula Chowanietz, Arno Deistler, Bernhard Forner, Christiane Bongartz, Wolfgang Herrmann, Claudia Lohmann, Juliane Hollender, Martina Schäfer and Michael Weber for their support during this time. The focus of the book was developed in a scientific way during my time at the University of Halle. The case studies were developed in cooperation with A.M. Ebraheem (who set up the first 3d modeling approaches of the Nubian Aquifer System) and doctoral students in the working group Hydrogeology and Environmental Geology, led by Peter Wycisk. I am very grateful for all the collaboration partners, especially Ahmed M. Sefelnasr (hydrogeological modeling of the Nubian Aquifer System, focus Egyptian oases), Ronny Lähne (hydrogeological modeling of the subrosion valley Unterwerra), Tobias Hubert (geological modeling of the Bitterfeld area), Reiner Stollberg (ongoing hydrogeological modeling of the Bitterfeld area, based on the hydrogeological model that is presented in this book), and Christian Neumann (runoff measurements of the creeks in the Bitterfeld area). Additionally, some diploma students contributed to the success of this work: Oliver Neef (local hydrogeological model of Bitterfeld), Raik Richter (interpolation of physicochemical parameters in the Bitterfeld area), Mark Pohlert (geological modeling of the town of Halle), Andreas Wollmann (detailed geological modeling of Bitterfeld), and Dirk Schlesier (geological modeling of the town of Halle). The work performed during the last seven years was made possible by the University of Halle. From the colleagues at the University I am very grateful for a vivid exchange of ideas to Michael Falkenhagen, Kurt Friese, Herbert Pöllmann and Ian Lerche. The colleagues Norbert Hauschke, Dorothee Mertmann, Jochen Mezger and Angelika Schöner were always open for a well-meant talk. The German version of this book was submitted and accepted as a habilitation thesis in 2008. The reviewers of the thesis were Peter Wycisk, Martin Sauter, and Gunnar Nützmann. I am thankful for several hints given to me that helped to enhance the thesis of this book.

Additionally I want to thank my parents and my sister for their support in several steps of my life and for the patience they brought up during the time to finish the book.

Content

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1 Introduction and terminological basics of hydrogeological and environmental geological models

The recognition of our environment, the prognostic “modeling” of future development and manual change for a better life are part of the existence of mankind. We have been analyzing our environment for thousands of years in various directions: astronomical observations are the best documented, but climatic and biological changes were also very important for the development of mankind.

In terms of water supply and the use of waterways, mankind has been changing the environment since the earliest times. Examples are cisterns, irrigation, water supply from Khanates and wells, changes to the shapes of rivers, and dewatering of wetlands, as reported by ASCE (1998); for some examples in Germany in brief see VORREYER (1987), and for the Berlin area see FORNER & GOSSEL (1996). Most often mankind did not have the ability to foresee all the results of these changes, but even without the active role of mankind, natural developments of the environment – especially changes in the water balance – have influenced the development of people. This was shown in detail regarding the desert area of North Africa by EDMUNDS & WRIGHT (1979), PACHUR ET AL. (1990), HOELZMANN ET AL. (2001), and KLITZSCH (1991). A fast prehistoric and historical development in Middle Europe was possible between and after the glacials. The analysis of processes and prognostic views for large areas – either of global changes or long-term developments – was most difficult in the past. The gap between the knowledge about processes and unintentional changes in the environment has been closed by recent developments in analyzing and modeling our environment with the help of computers. Models for parts of the water balance processes and chemical processes were developed very early. The complexity of waterbound processes is very problematic even today, on account of the high structural cross-linkage of the various solitary processes. Additionally, there is the problem of diversification in sciences. In particular, the compartments of the hydrosphere are examined by various branches of sciences. This leads to overlapping and competition among research activities, which can be useful for interdisciplinary work but can also be a hindrance in terms of terminology, quantification etc. The systematic consideration of connections between a modeling system of high complexity for parts of the water cycle opens the door to a transfer to fields involving the numerical modeling of processes beyond water balances, water flow and transport, and hydrochemical reactions.

1.1 Introduction and objectives

Computer models allow for the prognosis of distinct results of anthropogenic impacts on existing environmental systems. Environmental scientists and amongst them the hydrogeologists are able to estimate the impact on landscapes and water balances to a certain extent. VAN BERNEM (2001) expands the applicability of models to the fields of “Environmental Sensitivity Indices”, “Environmental Risk Assessment“, and „Environmental Impact Assessment“.

Models that are created with the help of modeling tools are images of reality that focus only on the aspects of certain questions. Most of the modeling tools are restricted to a distinct thematic part of the reality, so they are useful for many questions. They are highly specialized and detailed and can be used like toolboxes in several projects. In hydrogeology, each modeling tool is only useful for modeling a part of the water cycle and the cycles of other substances connected to it.

It is not adequate to use only one of these modeling tools for some purposes. A few examples will demonstrate this:

- All of the numerical groundwater models need a geological model that contributes structures and parameters by abstraction from the geological units. This model of slices and parameters is called a hydrogeological structural model. For most of the models, a first step is enough to create the structures in a plausible form but not in detail and this serves the necessities of the numerical processor in an optimal way.
- For water management questions as well as issues related to groundwater and drinking water protection, a groundwater recharge model and/or a soil water model besides a groundwater flow and transport model may be necessary. It is sufficient to parameterize the model with area-distributed and time-constant datasets in most cases. Only for sophisticated questions of the dynamics of a catchment area and for a thick unsaturated zone, high resolution area- and time-dependent datasets are necessary perhaps also with feedbacks from the saturated zone.
- Flooding aspects and drought scenarios depend on the coupling of groundwater and surface water models.
- Urban planning and technical planning sometimes need not only new distributions of parameters and/or boundary conditions but also the development of completely new modeling systems and tools.
- Transport modeling of chemical substances can be calculated only in reduced form by a transport model with advection, sorption and linear biological degradation. A coupling with chemical equilibrium models and species dependent biological degradation models is necessary in some cases.
- For the accurate calculation of risks of substances in the groundwater, it is not sufficient merely to look at the results of transport models, even if they are coupled with hydrochemical models. Questions of land use, the extraction and use of groundwater and soil, and biological and ecological development must also be analyzed and discussed.

Some of these partial models must be developed, maintained and used by experts in different disciplines. The interfaces and the interaction of the modeling systems must be clarified, preferably in advance.

The purpose of this book is to provide a theoretical and consistent systematic background for the interfaces. Examples are given to show the results of different coupling procedures. This also includes a view of different modeling concepts. The partial modeling systems of hydrogeology (saturated and unsaturated zone), geology and groundwater recharge are predominantly observed. Figure 1 shows that these are the dominant topics of the first part of this book. Chapter 4 is the central chapter, and here the focus is on the coupling of the modeling systems.

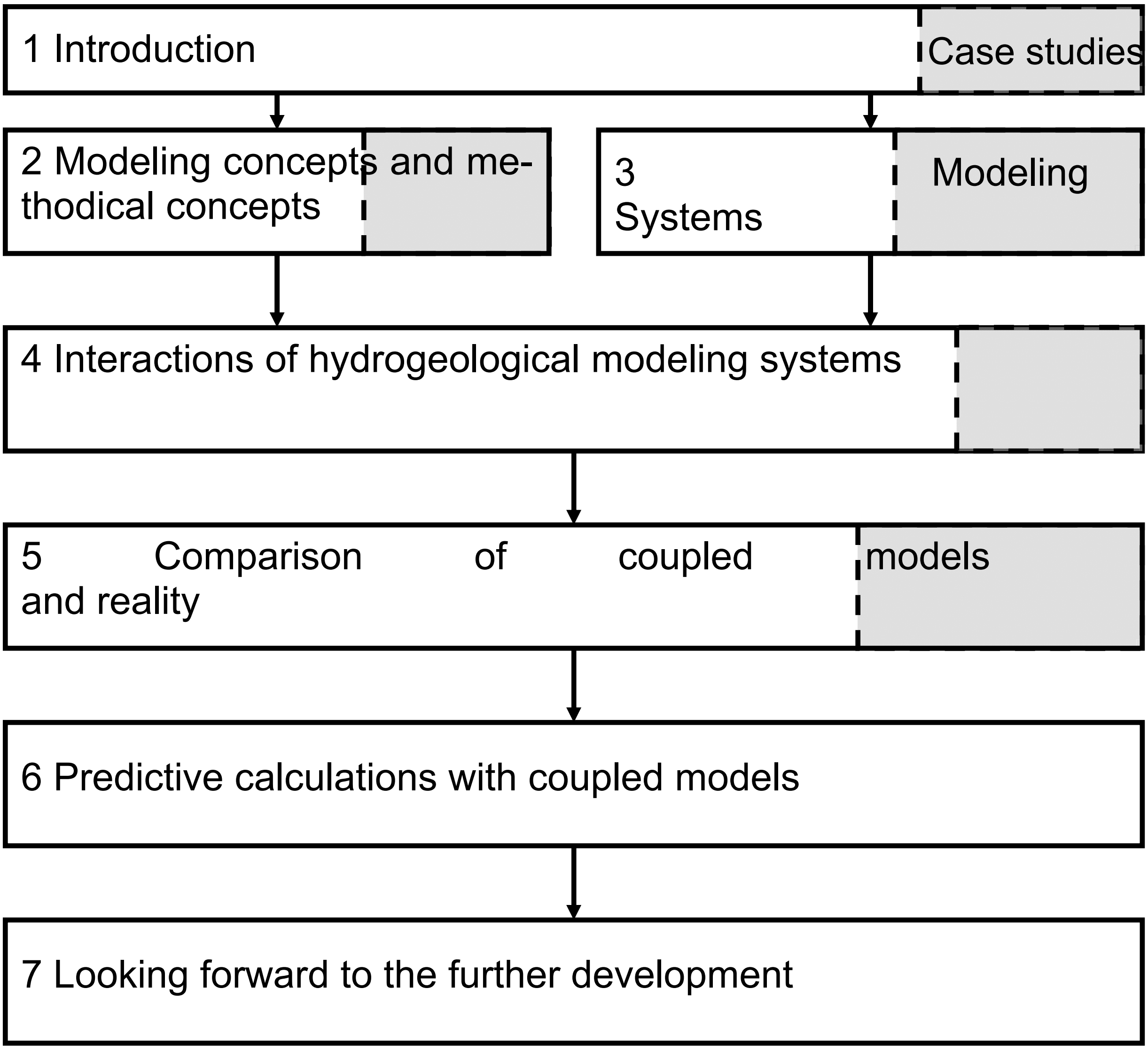


Figure 1: Structure of this book. The grey parts are examples of the estimated percentage of the whole chapters.

Chapters 5 and 6 will deal with the regular topics of hydrogeological modeling under the special aspect of coupling diverse modeling systems. This focus is chosen because coupled models require special treatment and additional criteria for calibration and for prognostic calculations. The concluding section attempts to give an overview of lines of development of model coupling and of the relevant interfaces.

1.2 Terminological basics

For better understanding the following definitions are given in advance:

- A **system** is an object that consists of several elements that are connected in a time-dependent way, and/or have area-based or multidimensional relations (BOSSEL 1994 and BUCHHOLZ 2001). Such a system is separated by defined boundaries from other systems, although there may be interfaces between the systems. Each element of a system can be regarded as a system of its own or as a part of another system. The superior system may lose its integrity by taking out a subsystem. BLUMENSTEIN ET AL. (2000) divide systems into simple and complex systems depending on the relations and the number of elements. Static and dynamic systems are marked by their time dependencies. The exchange between the system and the environment can be described as open or closed. The relations between the elements can be deterministic and/or statistic or stochastic. The behaviour of the system can be classified as stable or unstable. Figure 2 presents an example of the water cycles of Berlin with system elements from meteorology, hydrology, water supply, wastewater treatment and hydrogeology. The realization of a system with its elements and relations is, according to BUCHHOLZ (2001), a prerequisite for the creation of models. The setup of a model is achieved through a transformation involving additional steps into a mathematical model. According to DEATON & WINEBRAKE (2000) a system consists of

  1. Storage (or reservoirs),
  2. Processes, which determine the content of the reservoirs over time,
  3. Converters, which describe the rate of changes of the storages/reservoirs, and
  4. The interrelationships between reservoirs, processes and converters.

- **Modeling systems** are systems that are used only for the creation of models. The methods used in modeling systems are completely undefined and open. The modeling systems are blocks with systematic, structural, or spatial differences. These blocks/modeling systems, in our case in the field of hydrogeology, can be combined via definable interfaces, though they are certainly separated. Thus, they become elements of systems on a higher level.

- **Modeling tools** are realisations of modeling systems (BRASSEL ET AL. 1999). In most cases, these realizations are implemented as computer programs. The spectrum of these hydrogeological tools is able to cover everything from spreadsheets via GIS applications to highly specialized software, e.g., numerical groundwater flow modeling.

- **Models** are simplified and pragmatic images of nature. The term “model” is derived from the Latin word “modulus“ meaning drafts, examples, concepts, and plans. This common definition requires a more detailed definition and a description of related terms. On the one hand, BROY & STEINBRÜGGEN (2004) describe common data models in computer sciences as well as formal structures as models, as is the case in mathematics. On the other hand, in techniques and architecture, mostly static models are created. Science is dominated by highly dynamic models. KASTENS & KLEINE BÜNING (2005) describe different kinds of models: a model can be an image or the original. The original (model) as well as the image (model) can be real or abstract. From the field of geology, a real original may be a quarry with its layers, measured layer bottoms, or surfaces and tectonic slices. An abstract original would be the succession and lithostratigraphical structure of the theoretical existing sequence of layers. A real image could be a model of gypsum. An abstract model could be the diagram of fissures in a certain net. In logic, a structure S is a model of the logical formula F, if all formulas of F are valid for S (KASTENS & KLEINE BÜNING 2005).

- KAISER (2000) shows from his experiences with economic models that the modeling process must be as close to reality as possible in order to avoid a loss of information. He differentiates isomorphic models that are working without a loss of information from homomorphic models with a predefined loss of information. In practical hydrogeology, models are applications with parameters and boundary conditions of modeling systems that are implemented in modeling tools. Additional definitions and examples given by various researchers, such as BROCKS (2001) are not explicitly reported here explicitly.

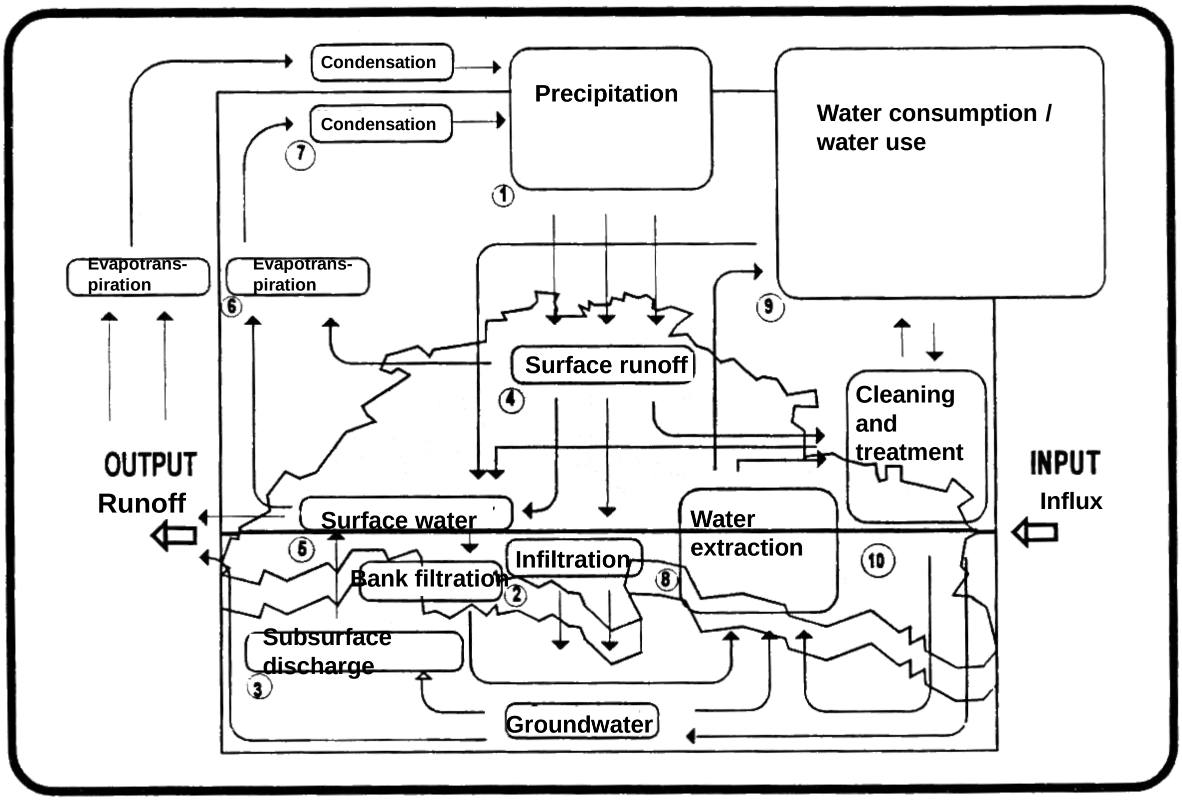


Figure 2: Example of a system constituted by several elements. The system elements are also systems. There exists a modeling system of very different quality for all of these systems. Also, modeling tools exist for some of them (after FORNER & GOSSEL, 1996).

The admissibility of the mapping of reality for the proposed purpose by the model is demonstrated via **calibration** and **validation.**

The application of the (mostly prognostic) boundary conditions and/or parameters leads to a **scenario**.

Modeling means the process of building models and scenarios using modeling tools. Figure 3 shows an overview of model development, with the purpose of the model in the central position. The purpose is significant for the admissibility of the modeling concept and the application of modeling systems. The modeling systems are decisive for applicable tools. The system development starts with the observation and analysis of the system and continues with the mathematical formulation until the model is realized through the means of the modeling tools. For complex models, one modeling system is not enough. Interfaces of these modeling systems and their systematic application play a significant role.

Regarding computer sciences HUBWIESER & AIGLSTORFER (2004) divide the modeling process into four steps. This approach can be used for the first parts of the modeling process in hydrogeology as well. All these steps are carried out in parallel, and in most cases they depend on each other. The first step is the outline of the model regarding the purpose, the spatial boundaries, and the temporal boundaries. The step of abstraction summarizes the exclusion of less-relevant details in the system structure. The idealization leads to a simplification of parameters and boundary conditions to ideal values. The description in the next step is a preparation for the use of existing modeling tools and for their application to the specific purposes.

In many cases, the approach of a descriptive model, the so-called word model of BOSSEL (1994) or, even better, the hydrogeological model of FH-DGG (1999), is sufficient. The conceptual model after BUCHHOLZ (2001) means a completely formulated modeling structure that is not represented in mathematical or physical terms. A similar formulation of the conceptual models is used by HILL ET AL (2004). Because of the quantification aspects the German term “Hydrogeologische Modelle” (FH-DGG 1999) goes beyond the formulation of conceptual models. The next step consisting of the mathematical formulation and (numerical) modeling is necessary for representative, prognostic scenarios. In this step, based on scientific laws, parameters and boundary conditions are defined in accordance with the modeling purpose in space and time. BUCHHOLZ (2001) defines a conceptional model as a mathematically formulated model with a very low resolution in time and space that does not fulfill the needs of a continuous model. This distinction will not be used further; instead, the definition of a conceptual model will be related to a process modeling structure in the sense of a conceptual model that is not formulated mathematically or physically.

The use of available modeling tools for several modeling purposes often leads to a coupling of these tools. The modeler must think carefully about the information that is received by one modeling system and about which information it will give to the next one. HINRICHSEN & PRITCHARD (2005) refer to the connection of modeling systems as a composite system. Focusing only on the technical aspects of data exchange between modeling tools is inadequate. This **coupling** of modeling systems can be carried out in several ways. Two of them will be mentioned here as examples:

The exchange of values for parameters and/or boundary conditions from one modeling system to the other is called **parameterization**. This procedure can be compared to the “call by value” of a subroutine or function in computer sciences. Another possibility may be that these values are changed before they are given to another modeling system or tool (“call by reference”).

A connection with **feedback** has another function: for each (or each predefined) time step, the results of the first modeling system are given to a second one that will give its results back to the first modeling system, which will calculate the next step. This kind of coupling can be compared to an iterative programming style in computer sciences. Another iterative approach is implemented in numerical modeling systems. There, the feedback is missing. These different coupling techniques can influence the results in different ways.

The approaches to coupling modeling systems can be very complex. This is the reason for this book, which attempts both to provide a systematic overview and to consider individual examples and the resulting rules.

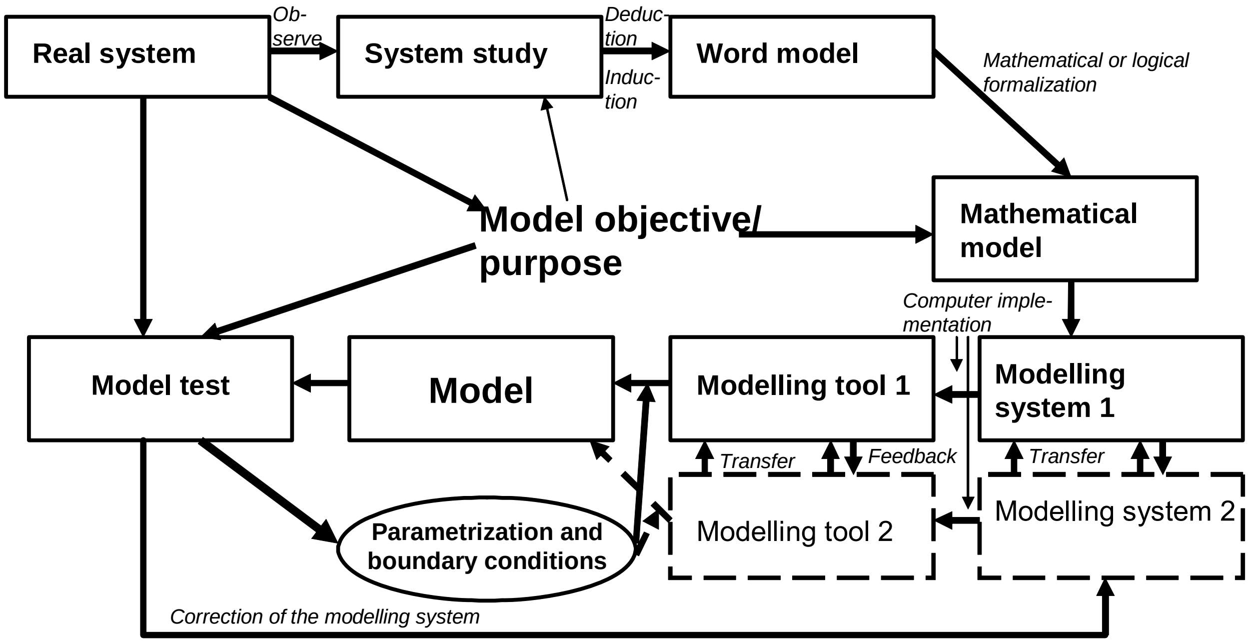


Figure 3: The process of the system analysis and model development (changed, based on BOSSEL, 1992). The purpose of the model development is in the center of the whole process. As more elements (and therefore also more modeling systems and modeling tools) are connected to a system or to each other the complexity of the whole system will becomes higher, according to BLUMENSTEIN ET AL. (2000).

1.3 Case studies

The theoretical analyses will be demonstrated by case studies from three numerical groundwater models, focusing on the methods of coupling. The model areas are shown in Figure 4. The succession of the models was chosen to describe the process of developing interfaces between modeling systems and the results of a systematic approach to this process.

- The model of the Subrosion Valley Unterwerra (a region around Eschwege in Hessia, Germany, see Figure 7) covers the widened valley filled with gravel and the adjacent hard rock area of the catchment. In terms of interfaces, the connection of hard and unconsolidated rock aquifers in one catchment is most interesting. The density of borehole locations is very high in the valley itself. This is an exemplary situation for hydrogeological investigation.
- The model of the Nubian Aquifer System (see Figure 5) refers to an area of two million km² in the Eastern Sahara (large parts of Egypt, the northern Sudan and the eastern part of Libya and the northeastern part of Chad). Besides the spatial extension, the temporal dimension of about 140000 years is characteristic. The connection of climatic changes with a numerical groundwater model is the central purpose. Additionally, the calculation of future scenarios is of political importance for the neighbouring countries. The model benefits from geological investigations that were conducted in this region in the last 20 years. The geological data serve in the model setup to create the structure of the numerical model and to support the model calibration with the necessary proxy data. Thus, the interfaces between geological and hydrogeological data are very diverse.
- The model for the area Untere Mulde/Fuhne (see Figure 6) investigates interfaces and coupling possibilities between very complex geological, hydrological, and hydrogeological models. Furthermore, the influence of open pit lignite mining on transport conditions in an aquifer of fluvial and glacial sediments of the Quaternary and Tertiary is investigated. The investigation area is situated in the middle of Germany (the region around Bitterfeld) with an area of about 320 km². The modeling purpose sets the temporal dimension to more than 150 years. This model is extremely interesting in terms of interfaces in the context of hydrogeological and environmental geological problems because the basic aspects of a high-resolution geological model and environmental investigations have already been carried out.

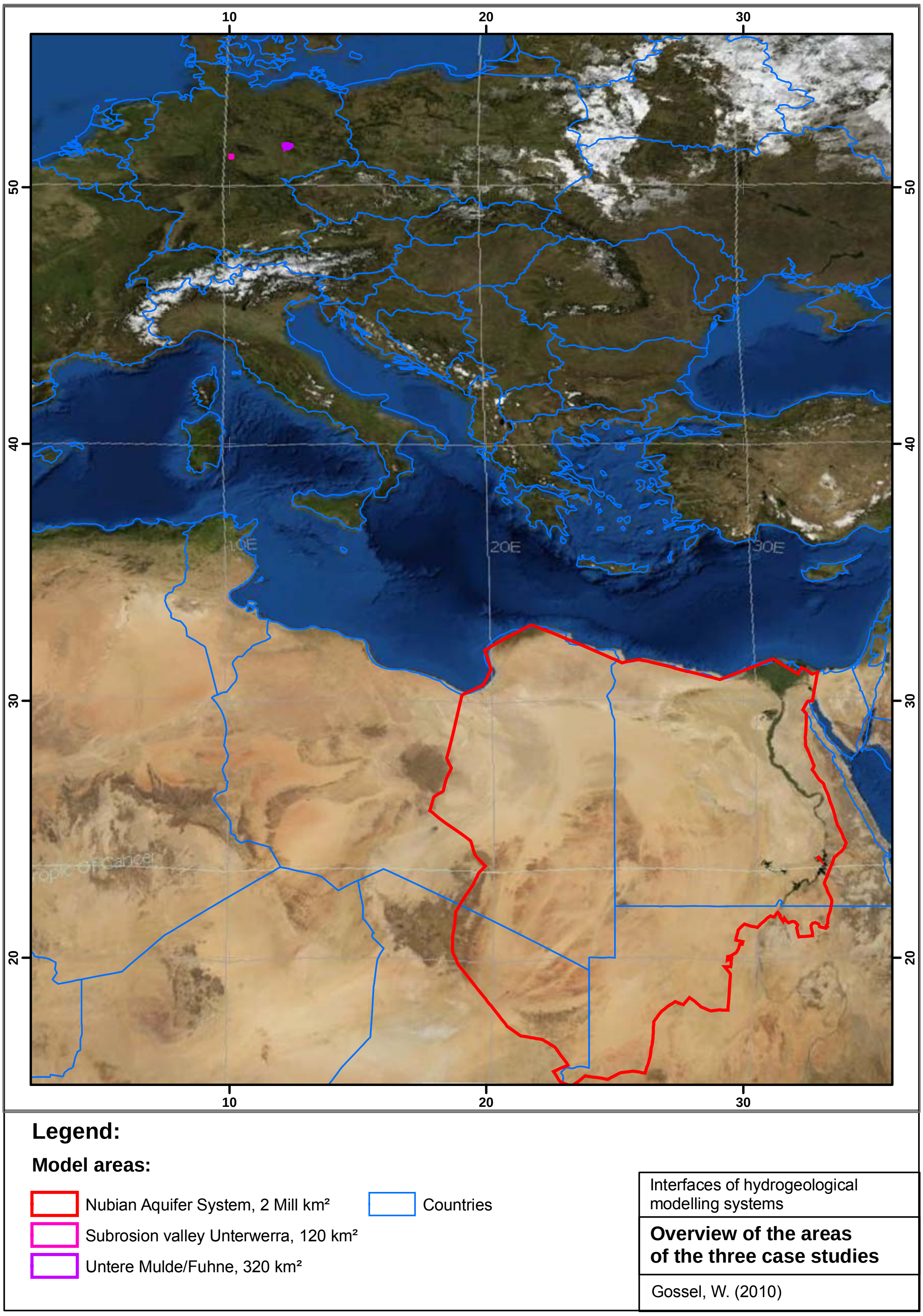


Figure 4: Spatial overview of the three case study areas based on satellite images (NASA 2007). The coordinate system is a geographical system (WGS 1984) with longitude and latitude values.

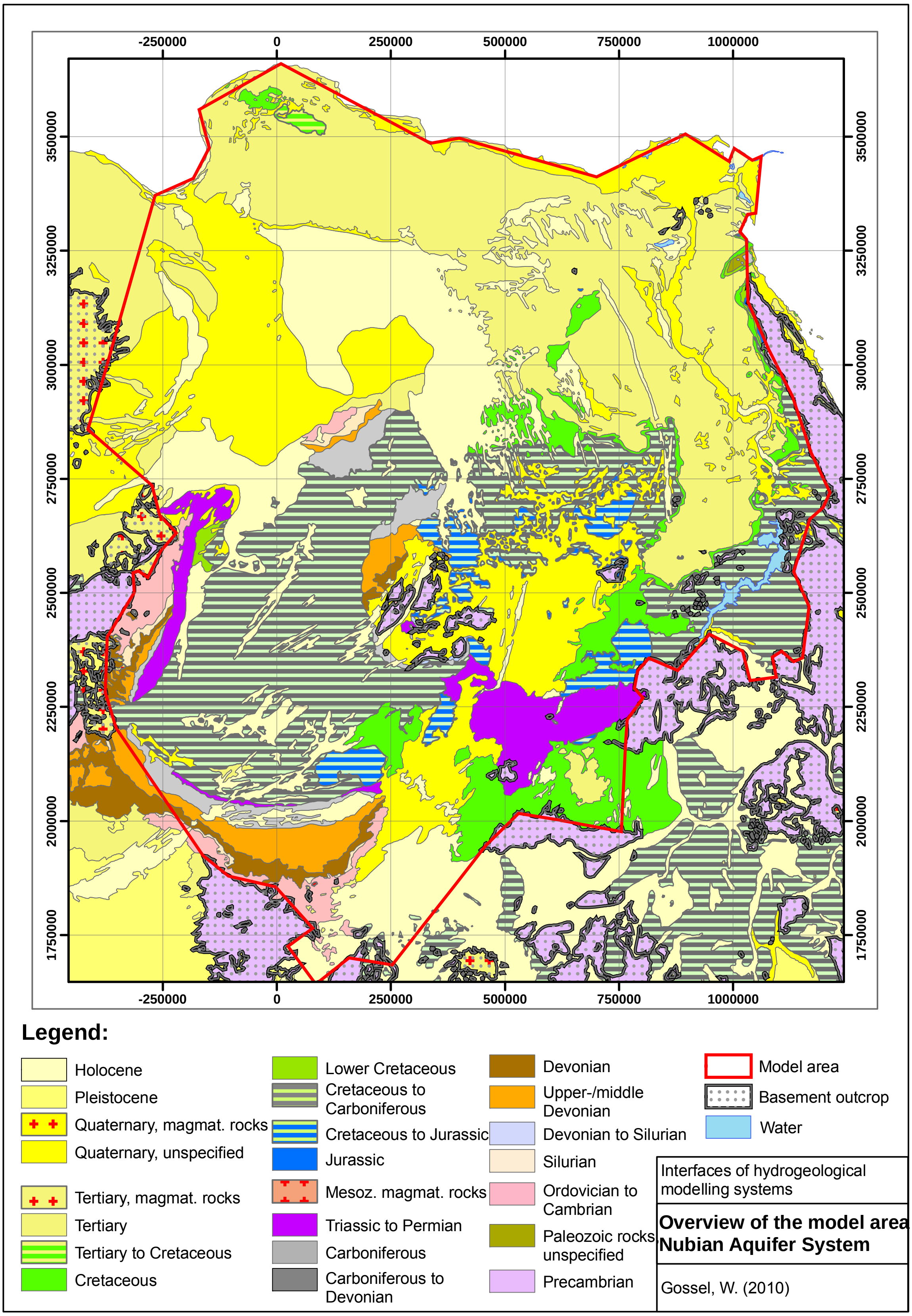


Figure 5: Overview of the model area of the Nubian Aquifer System. The model boundaries are defined mainly by geological patterns of the basement outcrop. To the north of the model area the Mediterranean Sea was chosen as a boundary condition. The database is the geological map (Conoco 1987).

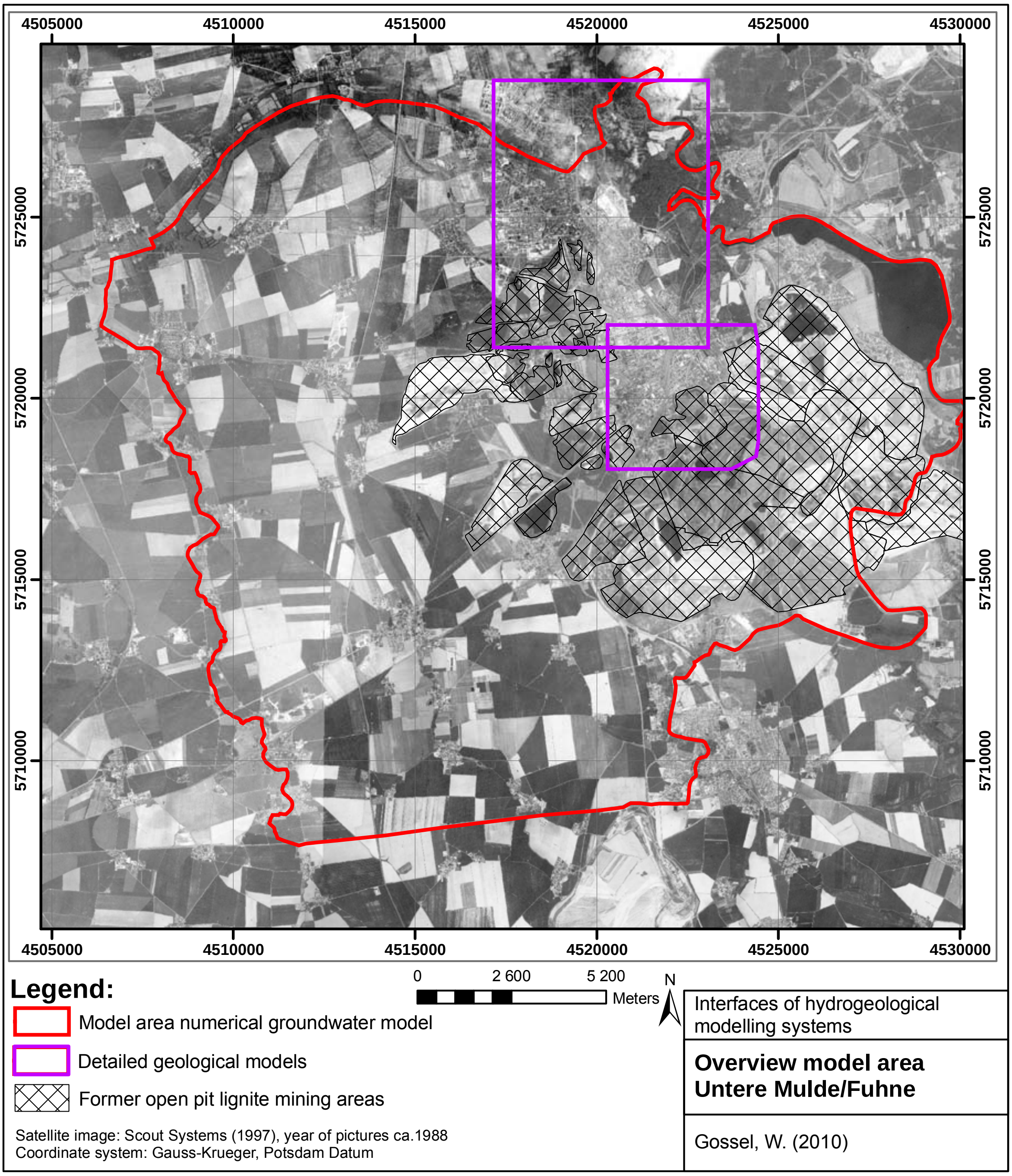


Figure 6: Overview of the Untere Mulde/Fuhne model area with the boundaries that were derived from hydrological and hydrogeological boundary conditions. The boundaries of formerly developed detailed geological models are also shown. Basic topographical data are based on a satellite image from the year 1988 (SCOUT SYSTEMS 1997). This image shows the outline of the open pit lignite mining in the latest stadium.

These studies were built partially with a very high resolution, adapted to the described purpose of the models. The background of this work is neither the purpose of the model itself nor the description of modeling tools. The interpretation of the modeling results – such as the assessments of risks, exposition routes, prognostic calculations of remediation possibilities, or the enlargement of water extraction capabilities – is not focused on this work. Only the differences in the use of diverse modeling solutions are investigated in detail based on a systematic approach. Thus, no comparison of modeling tools or elaborated models (all models will be developed further in the future) is given, but the directions of possible and useful developments are demonstrated in these case studies.

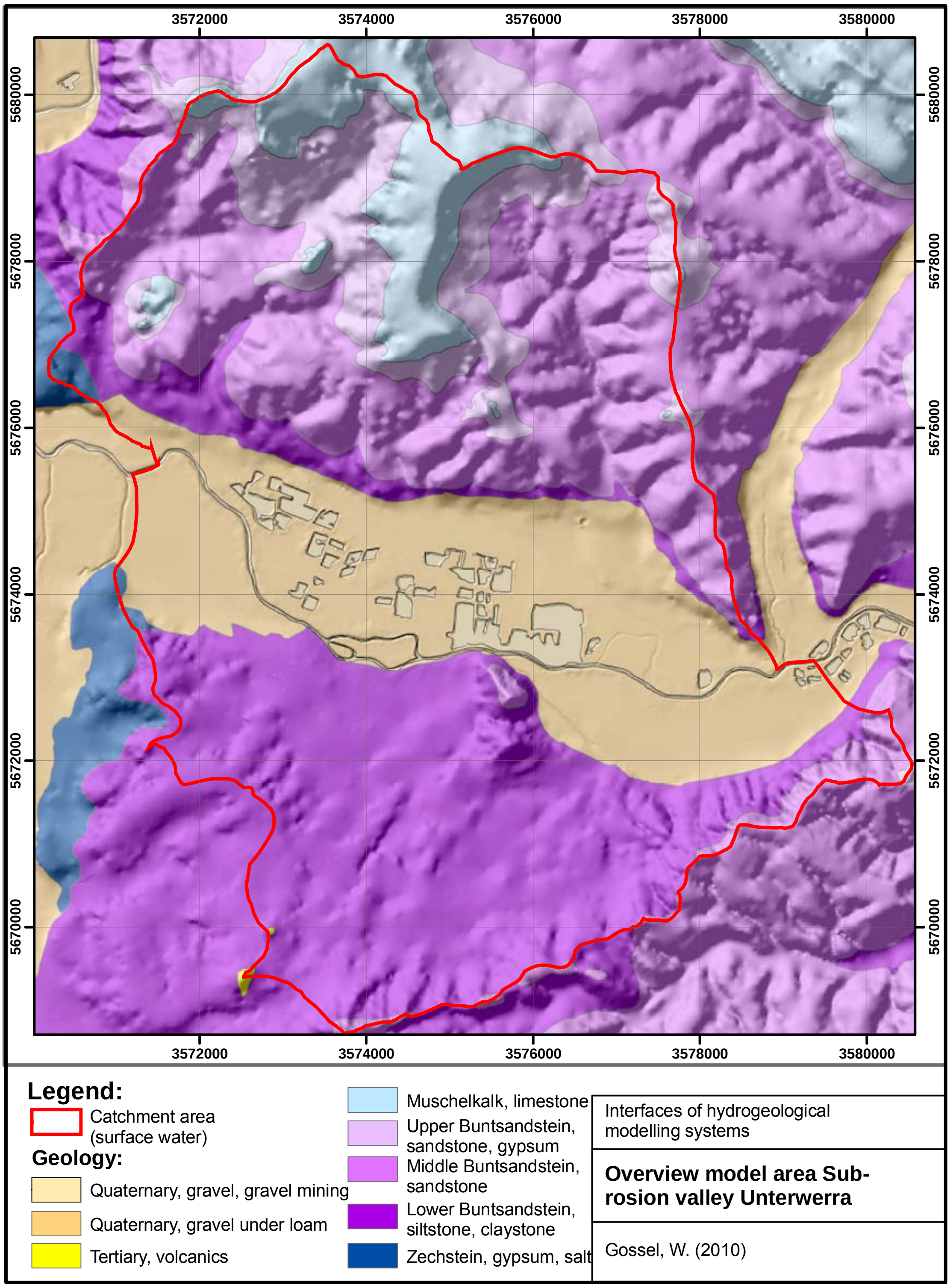


Figure 7: Model area of the subrosion valley Unterwerra with its catchment area. The model boundaries are defined by the surface watersheds. The database is the morphological model digitized from the isolines of the topographical map (HESSISCHES LANDESVERMESSUNGSAMT 1995, THÜRINGER LANDESVERMESSUNGSAMT 1997), shown as a shaded relief map, and the geological map recompiled from JACOBSHAGEN (1993).

2 Modeling concepts and methodical concepts

For BUCHHOLZ (2001), the modeling concept holds the central position in the modeling process. At this point

- Knowledge,
- Model assumptions, and
- The principles of model development and theory

are connected. The modeling concept therefore accompanies the whole modeling process. The chances and possibilities of a model are connected to the concept, which is also fundamental to model development. Several principles follow each other. They build a complex framework for the modeling process and for each single step, according to BUCHHOLZ (2001). Although these principles are very important, the quality of the modeling process cannot be estimated by an assessment of the proximity of the process to these principles, because some of them are exclusive of each other.

Principle of dominance: Only dominant processes are considered. The principle of dominance is supplemented by the **principle of simplicity**, which states the attempt to describe things as simple (and not as complex) as possible.

Principle of importance: The most important and necessary descriptive parameters and boundary conditions are identified. To fulfill the principle of dominance and the principle of simplicity, sometimes even complete processes are hidden in parameters, especially in hydrology. This leads to poorly formed process descriptions and problems in the scaling of processes.

BUCHHOLZ (2001) called the subdivision of the space into columns and horizontal “slices“ the **vertical/horizontal principle**. This principle is applied in the definition of the model space and in the internals of the modeling systems, but it loses its importance with the three-dimensional outline and the connection of modeling systems and partial processes. Nevertheless, this principle demonstrates the most important needs of the coupling of modeling systems. The **principle of topology** has almost the same meaning. The topology is oriented in hydrology according to the flow directions of the water.

The **principle of translation and retention** plays a role, in the internal structure of the modeling systems related to reservoirs and transport paths. This principle is supported by the **principle of linearity** which expresses the focus on advection processes.

BRASSEL ET AL. (1999) differentiates within the modeling concepts only the so-called macro concepts, which are used for very large systems and models of several economies (or of the whole world like the models of MEADOWS ET AL. (1972)), and micro concepts, which work with single economies. The concept of multiple levels serves as a connection between these main counterparts.

The **methodical concepts** comprise the basic structures of the modeling tools. Two of these methodical concepts must be distinguished according to the temporal components of their methods:

Static concepts are used for extensively time-invariant and therefore spatially oriented modeling purposes. Several of the very diverse case studies are geological 3D models (as described in WYCISK ET AL. 2002 and WYCISK ET AL. 2003), such as are most common in environmental geology, morphology, and landscaping.

Dynamical concepts focus on time-dependent modeling tasks, e.g. the transport of substances into the atmosphere, soils, or groundwater. Other objectives of highly dynamical models from hydrology and hydrogeology are the results of flooding or, even more commonly, the development of groundwater resources. The statement by BLUMENSTEIN ET AL. (2000) that geoscientific models are always dynamic does not hold true. Within the group of dynamic models, static models that rely on equilibrium (of fluxes, transport or reaction energy) should be distinguished from transient models, just as described by BLUMENSTEIN ET AL. (2000) in terms of geoecology and by KINZELBACH (1986) in regards to groundwater models.

In dynamic concepts, spatial aspects play a minor but remarkable role, unlike their role in static concepts. In contrast to the spatial aspects in dynamic concepts, the time dependency is not at all regarded in static concepts.

Both methodical concepts meet in the fields of hydrogeology and environmental geology, and they have their own specific demands and means of realization. Hydrogeology and environmental geology form, therefore, an important connection between static and dynamic modeling concepts. This will be discussed in chapter 3.

The models built on static modeling concepts often serve as donators of parameters for the spatial information base of dynamic models. In this approach, they are often implemented in a reduced form, but the definition of the interface must be carried out carefully.

The lines of development of the realization of the methodical concepts were completely different in the beginning.

Static spatial models were developed in landscape architecture, architecture, and engineering and they were rapidly enhanced. The adoption of the ready-to-use digital techniques for geological modeling started in the mid-1980s. The software was derived either from Geographic Information Systems (GIS) or from CAD applications. Static modeling tools were of great importance in the mining industry, for exploration as well as for the planning of mines. These tools were successfully enhanced and became real geological modeling tools.

Dynamical models were developed in the 1970s using on computers, e.g. in MEADOWS ET AL. (1972). In the beginning, they were one-dimensional. Hydrogeological models were developed in the 1980s, already having two spatial dimensions (2D models) (LUCKNER & SCHESTAKOW 1986, KINZELBACH 1986, DIERSCH 1984, MCDONALD & HARBAUGH 1983).

Both methodical concepts use a mixture of statistical methods and deterministic methods (or physical methods). Pure modeling systems based only on physical methods seem to be not applicable up to the present, and pure statistical methods do not fulfill the needs of predictive possibilities. The parts of both methods vary in different systems and tools. A classification of this nearly continuous set, as supposed by BOSSEL (1994), is not applicable. The implementations of pure physical or pure statistical methods seem to be the two ends of a line of possible methods.

Static and dynamical modeling concepts differ not only by focussing on different dimensions but also in the outline and in scales of the developed models: static models are local models of small scale areas with a high spatial resolution in most cases. Exceptions to this observation are reservoir models in mining, especially models of oil and gas reservoirs. On the other hand, dynamical models mostly integrate large areas and provide high temporal resolution. Global climatic models (GCMs) are exceptions to this rule. Based on these observations chapter 2 is structured according to Figure 8:

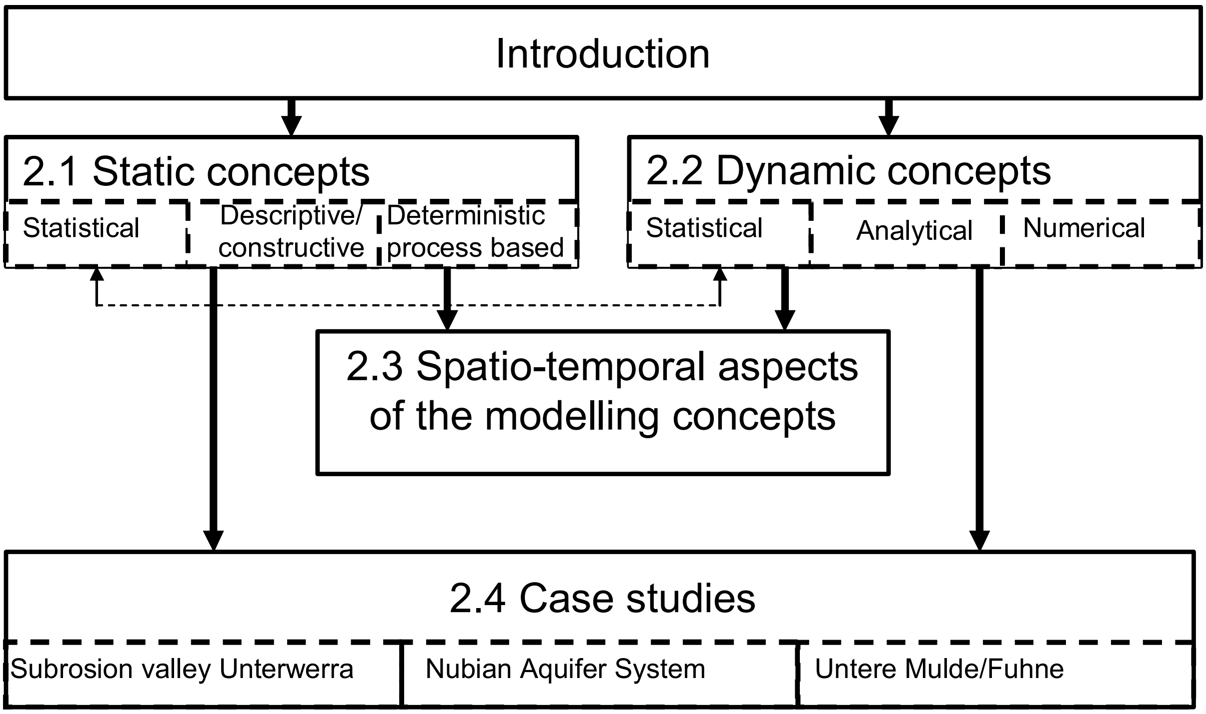


Figure 8: Graphical overview of chapter 2. For better orientation, this graphic is presented in the following subsections in miniature.

In terms of the considered database, the modeling methods vary widely.

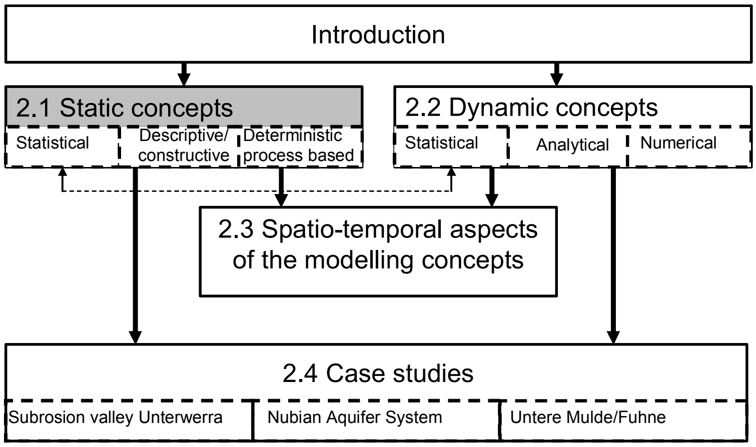
All statistical modeling systems rely on “hard” facts, especially in the case of hydrogeological models based on measurements, and a number of models with equal probability (realizations) are built on this database. The implemented methods are undetermined in the end. The different levels of a statistical analysis are described in detail in BLÖSCHL (1996). Geological knowledge can be adapted to the modeling process only by using enlarging the database using reasonable assumed “soft“ data. These soft data receive the status of hard data as a result of this approach. Compared to this, the methods for generating results are quite unspecific and can be applied to a great number of different spatio-temporal data.

In descriptive modeling systems constructive methods, which are able to consider also, are used. Thus, the statistical realizations are reduced according to knowledge. Various case studies show this for the extent of subsurface fluvial and glacial channels/gullies or through other descriptive principles. However, the constructive and descriptive methods are undetermined. That is why there is a theoretically infinite number of possible realizations.

Deterministic and process modeling systems use analytical mthods and numerical methods to build a model. These methods do not rely on measurements as much as the statistical or constructive modeling systems. For these models physical and deterministic principles and laws are most important. Deterministic techniques are definite techniques, i.e., from a given set of input data, only one set of output data results from the application of deterministic methods.

In the application of numerical methods, in most cases all three methods mentioned above are combined to develop a running model. The database must be created using statistical and/or constructive methods because the relevant data and measurements for running the model are not available in the necessary resolution. This database is connected by deterministic or physical methods to obtain definite results.

2.1 Static methodical concepts and methods in hydrogeology



Static concepts, static systems and static tools are very widespread in the field of modeling:

- Architecture: reproduction of buildings.
- Engineering: calculation of statics of buildings, description and calculation of tools, cars and other vehicles, etc.
- Landscape planning: modeling of the creative elements.
- Mathematical-statistical models: statistical and geostatistical methods were developed and can be applied for models in mining geology and economic geology. These modeling methods are also very important for the preparation of dynamical models, but the elaborated models are employing dynamical processes with static methods. This can be a problem if modellers are not aware of this difference.
- Assessment in environmental geology: assessment models that are based on spatial analyses, as discussed out by VAN BERNEM (2001). These models are used for sensitivity analysis, risk assessment and vulnerability investigation.

Structuring and analyzing datasets are the primary aims of static modeling. Several examples from hydrogeology and environmental geology are

- The three-dimensional distribution of aquifers and aquitards, including parameter distributions
- The analysis of potential flow paths in groundwater
- The calculation of groundwater recharge based on soil data, land use, depth to groundwater and climatic data
- The calculation of groundwater aquifer sensitivity, vulnerability or pollution risk based on a wide variety of hydrogeological, pedological and land use data
- Static exposure assessment of contaminations and area-based inputs of substances

Despite the wide variety of applications of static models, the dynamic processes are more important in hydrogeological projects. Therefore, the static concepts are not in the spotlight of the model development, but they are used and, in most cases, are needed for building the geological model and the structural model.

All static and spatial models result in a discrete form, i.e., in a non- or quasi-continuous model. Regular rasters, so-called GRIDs, are the preferred form of presenting results. An irregular triangular network is another possibility for representing quasi-continuous surfaces.

Three main lines of development for static spatial modeling methods can be distinguished. An almost continuous line of tools was implemented among these modeling methods:

- Statistical methods,
- Constructive or descriptive methods, and
- Deterministic or process based methods.

Also, the choice among these methods reflects the view of the scientist who is working with a tool that differentiates and subdivides sub volumes:

The theoretical background of all statistic methods is the production of multiple realizations with equal probability based on the same input dataset. For this procedure, widely continuous transitions from one model part (or volume) to the next can be preferred, carried out by spatial analyses and geostatistical interpolation. The complete heterogeneity (of the complete input dataset) serves as a measure of the heterogeneity of the realization.

Constructive methods reduce the statistically equal probable realizations according to additional information. This additional information is not a new “hard” dataset because it has already been used by the statistical methods. The information is added using knowledge of geologic principles, such as analogous behavior, genetic dependencies, and geometrical or spatial correlations. The use of proxy data that refer to the needed input data without the necessity of defining a deterministic function between proxy data and input data is most effective. In geological modelling, constructive methods lead to a sharp delineation of subvolumes that can subsequently be resolved by statistical methods in the parameter distribution in a hydrogeological model.

Process-based deterministic methods are very diverse and include analog and numerical methods. They are rarely used for the development of static models because they work with dynamic data and focus on dynamic processes in general.

The statistical methods make the best of descriptive input datasets and attempt to calculate at least a 2.5D distribution. These results are mainly descriptive as well. The applied statistical methods started with geometrical methods like the Thiessen polgygons (nearest neighbour method) and triangulations via spatially weighted methods (inverse distance weighted method) and developed into geostatistical methods with a preconditioning statistical data interpretation and analysis in advance of the main interpolation procedure, as is the case with kriging or conditional simulation. In the literature, the geometrical methods are mostly referred to as deterministic, in reality, though, they are not based on deterministic modeling approaches but rather on the geometrical relations of the sampling points.

KOLTERMANN & GORELICK (1996) present numerous case studies involving different modeling methods for the so-called hydrogeological structural model in their overview paper. This structural model is built by bounding surfaces (slices) and the according parameters like hydraulic conductivity and porosity, and it is used for the preparation of the numerical groundwater model.

Descriptive and constructive methods are mainly used for the development of geological models. For this purpose, a precise stratification of the input data is needed. This is difficult when there is a lack of borehole data, e.g. when only geophysical data are available. It is easy when there are geological maps and detailed, analyzed borehole data. The object is to obtain separated geological volumes. Constructive methods already use interpretations for the input data. The subsequent modeling methods are also much more interpretative than the statistical methods. The hydrogeological models with conceptional character as considered in FH-DGG (1999), ("Hydrogeologische Modelle") are also descriptive models.

Process-based models are implemented mainly for genetic research questions. Therefore, their field of application is reduced at present to reservoir exploration and to some studies in environmental geology. For the application of process-based methods, knowledge and deterministic description of the underlying processes are essential.

According to its definition, the static modeling concept cannot directly serve for predictive modeling tasks because such modelling concepts are time invariant. Nevertheless, the realizations (models) reveal possible development strategies. As an example from hydrogeology, the structural (and behind that, the conceptual) model may outline connections between aquifers and, therefore, possible flow paths for contaminated groundwater.

The following chapters focus on research topics and examples from geology, hydrogeology, environmental geology and hydrology.

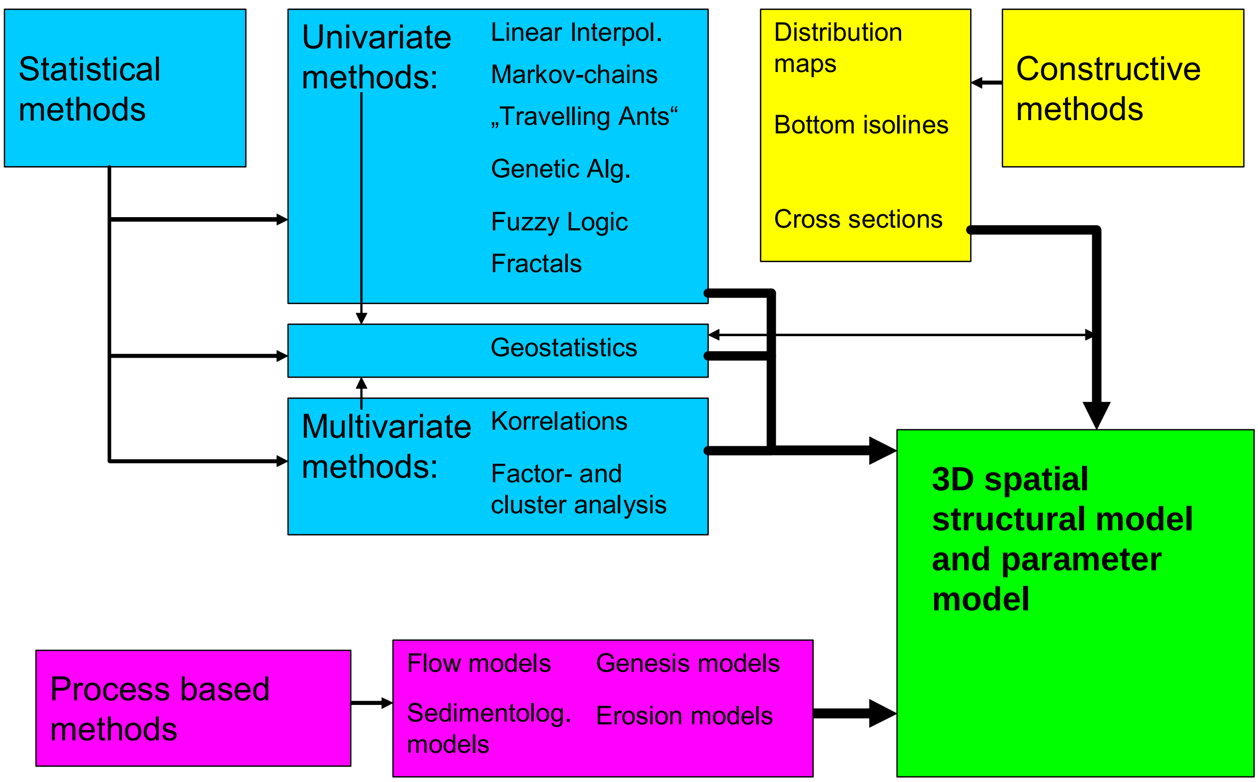


Figure 9: Statistical, constructive, and process-based methods in static modeling.

2.1.1 Statistical methods

The statistical methods are divided into univariate and multivariate methods. In geosciences, univariate methods focus on the estimation of parameters in spatial dimensions, whereas the multivariate methods are used to identify dependencies between parameters. This may serve for a calculation of an enhanced distribution. Not spatially oriented univariate and multivariate methods are not considered any further in this work (as there are statistical values like different means (arithmetic and logarithmic mean, median), and kurtosis, and also factor and cluster analysis).

In the beginning, spatial statistical methods focused on the calculation of 2.5D surfaces. Via a connection of the surfaces and the closing into volumes, 3D volumes are established. These volume bodies allow for far more evaluations, analyses and interpretations than do the surfaces.

For hydrogeological models, the way in which the distribution inside a volume body is handled is most interesting. The question behind the necessity of obtaining a parameter distribution in a model structure is related to real multidimensional interpolation techniques. In a multidimensional context, this topic becomes even more complex. WACKERNAGEL (1995 and 2002) presents possibilities of co-kriging methods, but these techniques have so far been applied only to 2.5D cases studies.

Borehole information is a primary source of data for geological statistical models. This part of the database is the same as the database for constructive methods (see chapter 2.1.2). The introduction of expert knowledge is very restricted. The insertion of virtual boreholes or the import of geophysical data by technical means is possible for additional solutions.

The statistical methods implemented for the interpolation of geological structures or hydrogeological parameters are mostly geostatistical methods. In the first step, they propose a spatial statistic that goes far beyond the means of non-spatially oriented statistical analysis. The variogrammetry opens a door to the knowledge of the scientist. DAVIS (1986), DEUTSCH & JOURNEL (1992), SCHAFMEISTER-SPIERLING (1990), SCHAFMEISTER (1998), and SCHAFMEISTER (1999) describe methods of elaborating adopted variograms, especially for sub-areas or zones. This may be effective for geological patterns or the special behavior of hydrogeological parameters. This topic will be discussed later. The geostatistical interpolation is carried out after a detailed spatial statistical analysis.

Along with geostatistical methods, additional methods can be used for spatially oriented statistical analysis and interpolation:

- Markov chains were used by LUO (1993) for the one- and two-dimensional interpolation of borehole profiles and for the estimation of ore contents in mining geology and economic geology. This method can be adapted to the interpolation of hydrogeological parameters as well.
- Fractals are increasingly being introduced to hydrology (KORVIN 1992, BLÖSCHL 1996). In hydrogeology, these interesting methods for the generation of static models are unfortunately not yet widespread. DIMRI (2005) presents several case studies from geophysical models that could serve as examples for the generation of hydrogeological models, especially for parameter distributions. KORVIN (1992) calculates distributions of the permeability of hard rocks that are dominated by fractal distributions of clay minerals. HECHT (2004) applies fractals to the grain size distribution and to the patterns of faults and fissures; this may be useful for hydrogeology in areas with hard rock aquifers.

- Genetic algorithms (DAVIS 1991) and simulated annealing are additional methods that promise successful generation of geological structures. In the meantime, these methods have been introduced to geology research only for some small experiments, though they have been established in other scientific disciplines for several decades.
- Fuzzy logic also allows for a setup of geological structures. NORDLUND (1999) shows how sedimentological models can be developed for exploration applications.
- The algorithms of the “Traveling Ants“ method (DORIGO & GAMBARDELLA 1997) were not adapted to geological research, though could prove useful. Several case studies in geography show their potential for application to spatial research topics.

Comparisons of the geostatistical and geometrical methods were carried out and demonstrated by several authors including SCHAFMEISTER-SPIERLING (1990), HEINRICH (1992), and KOLTERMANN & GORELICK (1996). An overview and comparison of more than 40 interpolation methods is given by LI & HEAP (2008). SINDAYIHEBURA ET AL. (2006) compared the results of several commercially available tools based on profiles across complicated structures and difference maps of the values and the first derivatives (slopes).

2.1.2 Descriptive and constructive methods

Constructive methods for a spatial geological modeling rely on the classical workflow of the construction of vertical cross sections and horizontally oriented distribution maps. Therefore, they can be called descriptive. In this modeling, not only stratigraphical and lithological data but also facial and genetic concepts can be analyzed. This can significantly enhance the model according to the knowledge of the scientist. The basic methods of the application in the field of geology are described in detail, such as in GROSHONG (1999). The realization of these methods with the help of computer sciences is described for several modeling approaches by WYCISK ET AL. (2002), BECKER-HAUMANN (2005), and SOBISCH (2000). These methods produce a dense dataset of hard and soft data that can be analyzed by relatively simple statistical methods (a triangular irregular network) to obtain separating surfaces or bottoms of geological layers.

Whereas statistical methods have changed rapidly and fundamentally in the last few decades (especially in geostatistics), the constructive methods have remained constant, only changing according to the use of digital technology.

Constructive methods are very sensible regarding the changes of the database, and this is a serious disadvantage when comparing such methods to geostatistical methods. With some new boreholes, usually additional cross sections have to be constructed and the whole modeling process starts again. This takes much more effort and time than merely interpreting a new variogram and interpolating again.

2.1.3 Deterministic or process-based methods

Process-based methods are established mainly in sedimentology to generate static geological models. From the systematic point of view, they stand between static and dynamical modeling concepts because, in their scope, they use the calculation of dynamical processes for the generation of static models. HSÜ (1989) compiles already fundamental calculation methods and LEE & HARBAUGH (1991), MARTINEZ (1991), WENDEBOURG & ULMER (1991), TIPPER (1991), and CSIRO (2004) present computer programs or modules of computer programs that describe fluviatile and clastic marine sedimentation scenarios as well as chemoclastic and organoclastic sedimentation. Diagrams of mineral parageneses were developed and computer programs have already been adopted for magmatic metamorphic processes (GUGLIELMO 1991).

BRÄUER (2002) shows how turbulent hydrodynamical flow processes can be modeled by fractals. This also explains the sedimentation processes that are connected to these flow processes and the distribution of hydrogeological parameters in aquifers which consist of fluviatile sediments. The calculation of fractals as the main statistical method uses, in addition to the statistical values, values that are derived from the knowledge of sedimentological processes.

MUIR WOOD (2004) derives numerous geotechnical parameters and engineering geology parameters using empirical modeling from geological process understanding. These empirical calculations and models, which were derived from laboratory measurements and in situ measurements, are based not on knowledge of the geological genesis of the rocks but on a few assumptions related to parameter distributions.

ADAM (2003) goes far beyond these first steps in the analysis of distributions (“patterns“). He describes the processes that lead to these distributions with mathematical and physical basic laws and principles. Unfortunately, his examples are disorganized and, furthermore, are of little relevance to hydrogeology. However, the basic idea of explaining natural distributions by a mathematical description of the background processes is a very important contribution to future geological and hydrogeological research. This approach can enhance the pure statistical or constructive analysis through the addition of geological knowledge.

Geological processes are mostly irreversible, and they are very long-lasting. The discontinuous parts of geological processes make things even worse. Consequently, many processes cannot be carried out as experiments in the laboratory. The process-based descriptions of parameter distributions are thus not easy to develop. Conceptual models are a first attempt at overcoming some of these problems, even systematic and theoretical problems, but they cannot as yet solve the problems of obtaining better parameter distributions.

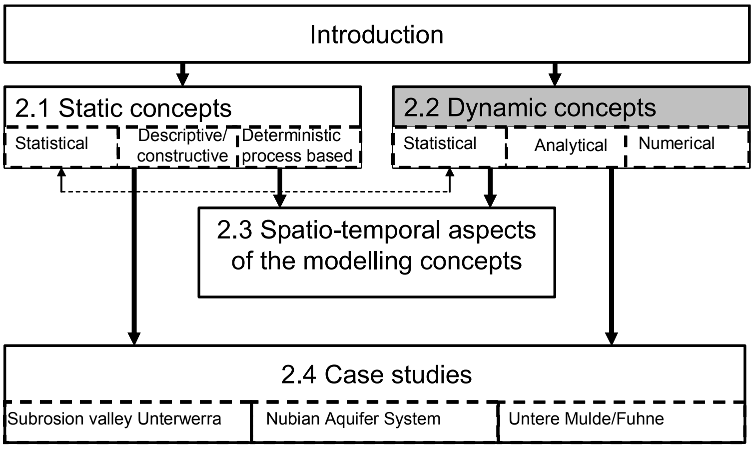
Modeling of soil erosion and sedimentation processes can be performed based on the Universal Soil Loss Equation (USLE) (WISCHMEIER & SMITH 1978). Today these equations are used only for the calculation of soil erosion, but they could be developed into a major input for the additional calculation of hydrogeological parameters in sedimentary rocks. Meanwhile, these modeling methods are partly integrated into GIS tools and they are ready for use in practical applications.

In hydrogeology, steady state numerical groundwater models can be regarded as links between dynamic models and static models. They are process oriented, but they rely on structures, parameter distributions, and boundary conditions that must be elaborated with static and constructive methods. Their fundamental starting points are flow nets. The flow models are derived from this basis.

In hydrochemistry, the modeling systems of equilibriums play a role that is comparable to the role of steady state models in hydrodynamics. They are also a special case of dynamic models. For hydrochemical modeling, kinetic modeling approaches must be separated from equilibrium modeling.

For the application of process-based models, determining which processes should be regarded in which scales is crucial. The observed and investigated processes must be classified as characteristic scales. The input values can be adapted to the “area of interest”.

2.2 Dynamical methodical concepts and methods in hydrogeology



Dynamical methodical concepts have long been applied in hydrogeological modeling. Initially, the solutions were based on analytical methods e.g. the analysis of aquifer tests. Basically, the famous experiment of Darcy is a dynamical solution, though it was carried out as a steady state experiment in general.

For the dynamical methodical concepts, a classification according to the applied methods is possible

- Statistical methods often neglect the process structures and focus on the statistical dependencies. The methods, that deserve mention herein, are time series analysis (trend analysis, periodicity analysis and autocorrelation analysis), correlation analysis, and factor analysis and cluster analysis. This also offers a hint regarding the underlying processes, as described in GOSSEL (1999) in relation to processes of groundwater recharge and the interaction of groundwater and surface water. Statistical methods have a special importance in hydrological catchment modeling (e.g. DYCK ET AL. (1980b)).
- Analytical methods constitute a classical field of work in hydrogeology, especially in terms of the calculation of parameters. The most prominent examples are aquifer tests, open-end tests, and slug and bail tests.
- In groundwater studies, models based on numerical methods have dominated the hydrodynamical and hydrochemical modeling for about 10 to 15 years.

The statistical methods in particular are used in static and dynamical methodical concepts. They also comprise an extensive mixture of methods that reflects their great influence on hydrogeology. In dynamical concepts, they are more or less static in the analysis methods (e.g. correlation analysis). Most of the statistical methods can be used in static concepts as well as in dynamic concepts.

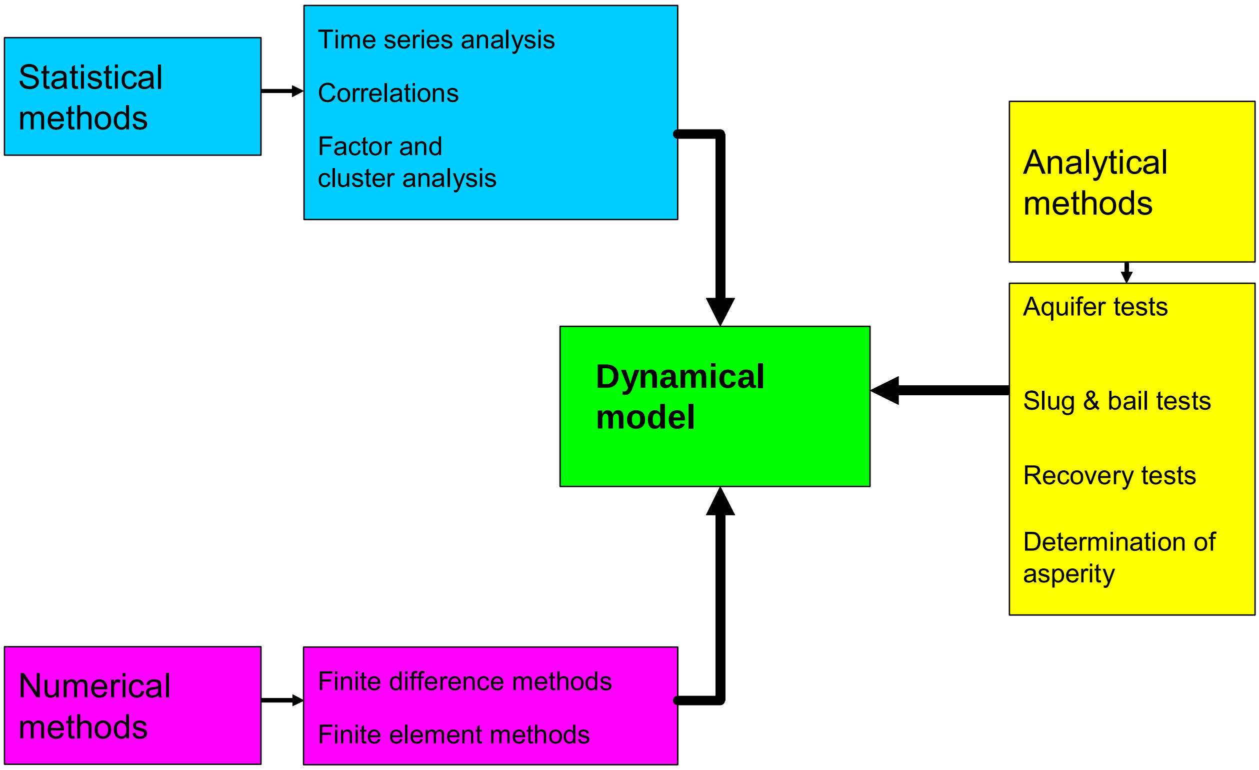


Figure 10: Statistical, analytical, and numerical methods in dynamical modeling.

2.2.1 Statistical methods

Statistical methods are predominant in the hydrological investigation of catchment areas and in the analysis of discharge and hydrographs. The methods described in DYCK ET AL. (1980a) and DYCK ET AL. (1980b) are in most cases stochastic methods including numerous statistical methods. For the dynamical investigations, the time series of hydrographs are analyzed, but time-dependent concentration measurements are also of great interest in hydrology as well as in hydrogeology. The main stages of a time series analysis are trend analysis, analysis of periods, and autocorrelation analysis. Special requirements are set in these methods because of the singularity or missing reproducibility of hydrological or hydrogeological events and because of the irregularity of sampling. The requirements of the sophisticated statistical methods can be better fulfilled through increasing automation and through the increasing reliability of auto-samplers in the field. In GOSSEL (1999), methods for statistical handling of unevenly or irregularly sampled data are described. These practical methods are very computationally intensive. In hydrology, the time series of discharge, with flooding and drought discharge, are analyzed in particular, but meteorological data – e.g. precipitation data (BARDOSSY 1993), temperatures, evapotranspiration data and concentrations of gases (e.g. CO_2) in the atmosphere – are also focused on. The problems to be solved are connected not only to trends, periodicity, and autocorrelation but also to statistically significant predictions of flooding events or droughts with the corresponding discharge rates or water levels.

2.2.2 Analytical methods

The analysis and calculation of hydrogeological parameters is a classical field of application for analytical methods. Analytical description and calculation of a time-drawdown analysis of aquifer tests or slug&bail tests are the most important examples of these methods. These methods are mostly bound to ideal conditions owing to their complexity, and therefore they cannot be applied everywhere. Some of these restrictions will be mentioned here although the development and enhancement of analytical methods greatly expanded the fields of application as described in BRUGGEMANN (1999):

- The calculations are mostly only applicable to homogeneous aquifers.
- Isotropy is generally a precondition.
- The calculations are only applicable to relatively simple experimental test arrangements. Solutions for complex arrangements are only available from analog considerations.

The crucial factor in the enhancement and development of new methods was the application of computer tools. Very complex equations could be solved with these tools. Simultaneously, new possibilities for visualization of dynamical processes developed.

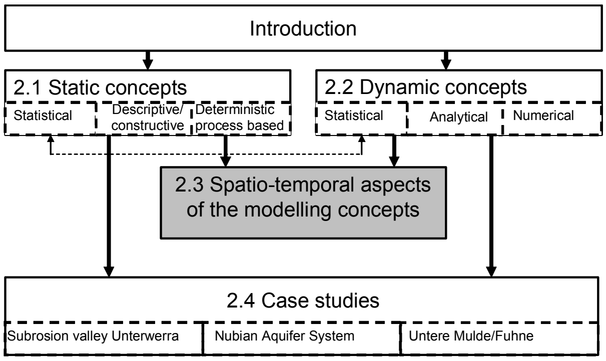
2.2.3 Numerical methods

Since the mid-1980s, numerical models have been applied to the modeling of hydrogeological systems. LUCKNER & SCHESTAKOW (1986), KINZELBACH (1986), DIERSCH (1984) and MCDONALD & HARBAUGH (1983 and 1988) transferred methods from engineers and enhanced them for hydrogeological purposes. Using these methods, they solved the highly non-linear equations that came from the combination of the continuity equation and Darcy's law. Solving the equations iteratively and putting them in linearized form were the most significant steps. Numerical methods were also adapted to the development of global climatic models and runoff models. ROBINSON (2001) describes the exchange between atmosphere and terrestrial and extraterrestrial energy sources primarily in an analytical form, but he then converts these equations via discretization to linear equations. The climatic and hydrological models of CLAUSSEN & GAYLER (1997), KUBATZKI & CLAUSSEN (1998) and DÖLL & FOHRER (1999) cannot be solved without numerical methods.

Numerical methods are based on the principle of linearization, i.e., solving non-linear equations with discretization and iterative handling. For this purpose, space and time are cut into small pieces, for which the assumed linear solution with spatially constant parameters and boundary conditions is tolerable. There is an analogy to the spatial interpolation methods described in chapter 2.1.1. These interpolation methods are used for the setup of a wide range of dynamical numerical models. Numerical methods depend mostly on interpolation tools during their application in modeling systems, modeling tools, and models. The connections between parameters, boundary conditions, and the results of the models are not linear, despite the discretization and linearization of the equations. This makes the calibration of models difficult and the solutions are usually not unique.

In most modeling tools in contrast to spatial modeling automatically adaptive methods are used for the temporal discretization. These methods are oriented to the changes of the resulting values, taking place from one time step to the next. The reasons for these changes are normally different boundary conditions and/or parameters. If certain criteria that are defined by the user are exceeded, the time step length is reduced; if a criterion is fulfilled this criterion is enlarged. This happens only when there are no additional user-defined breakpoints, e.g. the need for results at a certain predefined time.

2.3 Spatio-temporal aspects of the modeling concepts



Concerning the dimensioning of concepts the static concepts can be classified into 2D concepts, 2.5D concepts, and 3D concepts. Two-dimensional concepts are useful for all information-based models, in whigh areas are touched, i.e. most models in environmental geology. Concepts with a focus on the surface or other spatial interfaces are adapted to 2.5 dimensions. Real 3D concepts are applied to spatially differentiated questions for which geological structures are of high importance. In hydrological modeling, the third dimension is only useful for the differentiation of processes according to the vertical-horizontal principle and to the topological principle.

In static models, the horizontal dimensioning of the model area plays a minor role. The information value of a model is not affected by the dimensioning if the purpose of the model is taken into consideration.

The dimensioning of geological models should focus on the extent of the geological bodies. Therefore, a detailed analysis is necessary before outlining the model boundaries.

The spatial scale is more important in hydrology than it is in geological and hydrogeological modeling. Furthermore, the spatial and temporal scales are connected to each other:

- Up to areas of several hundred meters, the scale is called local.
- The scale of landscapes reaches about 10 km.
- Large catchments are represented in regional scales up to about 1000 km.
- Larger areas are continental scales. This scale, as well as the smaller global scale, is of minor importance in hydrogeology but is of great importance in climatic research.

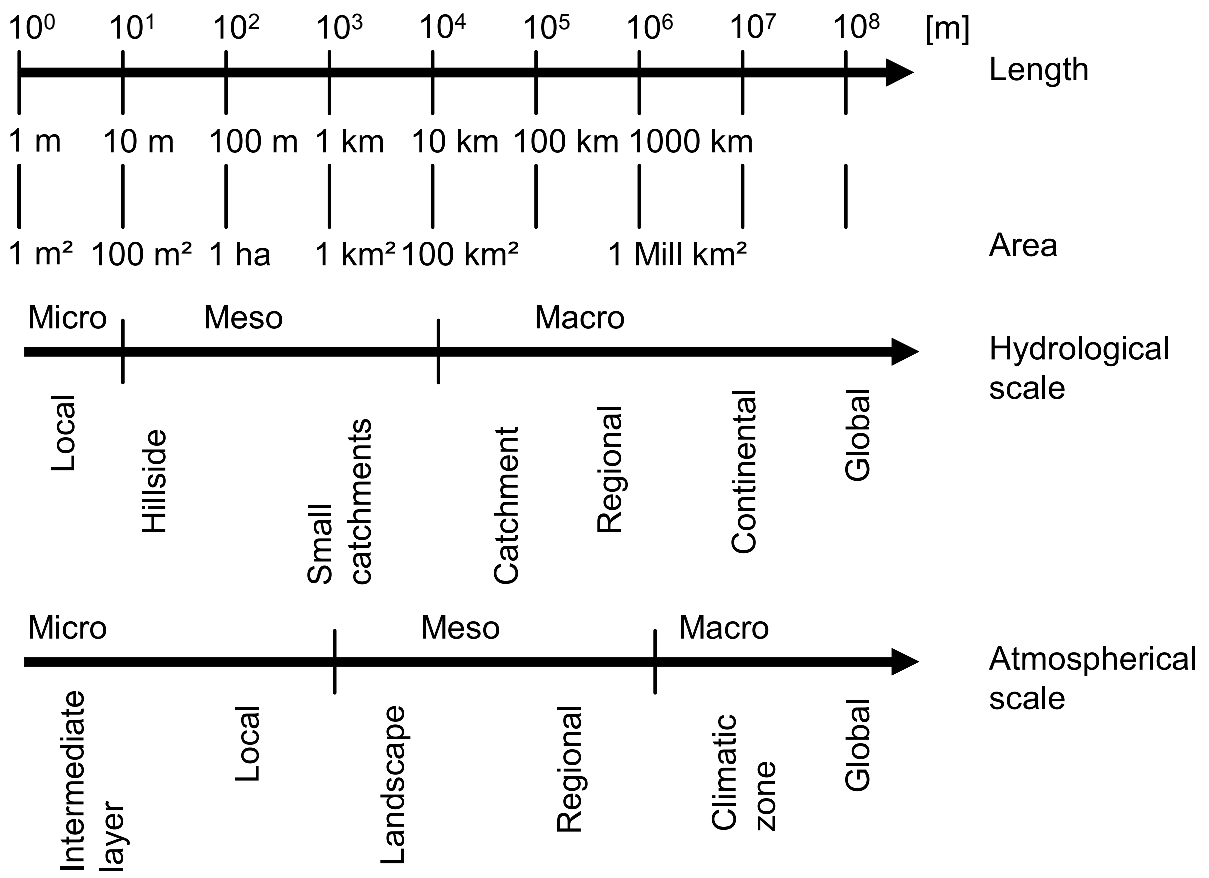


Figure 11: Spatial scales in hydrogeological modeling (changed according to BRONSTERT ET AL. 2005).

In addition to the scales described above, the following types of scales must be differentiated for the characterization of spatial dimensions in modeling:

- Process scale,
- Sampling scale, and
- Model scale

The spatial values characterize a model spatially and should be adjusted to each other: the dimensions of the investigation area, the density of sampling points or the sampling distance, the range of samples and the discretization of the resulting model. All these values are dependent on and connected to the three scales above, but in the end the process scale dominates the sampling scale and the model scale.

In hydrogeology, as well as in hydrology, the dimensioning of models must fulfill criteria that are not present in geology. The outline of hydrogeological and hydrological models is dominated by the boundary conditions that must – in the case of hydrogeological models – be derived from the flow net of the conceptual model in the startup phase of model development. For the definition of boundary conditions, also geological aspects – e.g. the distribution of aquifers – should also be considered. However, in most cases hydrological boundary conditions are predominant. The best example of this is surface water (mostly rivers) with a defined water level and/or a defined inflow or outflow, as in the case of watersheds. For watersheds, a non-flow boundary condition can be assumed.

The discretization of the investigation area is more important than the scale of a geological or hydrogeological model. As with GeoInformationSystems in 2D space, three concepts are used internally for the 3D geometries, as described by HERTER & KOOS (2006) and BRINKHOFF (2005):

Discrete volumes are domains of statistical modeling methods. They are comparable to rasters in GISs and consist of cubes or prisms. This is why the local resolution is the same for all sub-areas. Their design is described in detail in BAUMANN (2005) and BRINKHOFF (2005). Besides regular rasters, the so-called quadtrees and R-trees can be implemented for a better spatial acquisition and representation.

Geometrical concepts provide a better representation of geological volumes. This is supported especially (but not always) by constructive modeling methods, which are similar to the vector-based but non-topological geometries in diverse GISs and in several extensions of CAD systems. THOMSEN ET AL. (2005) demonstrate the possibilities of modeling geological volumes with appropriate tools, especially for these geometrical concepts but also for the topological concepts described in the next passage.

Topological concepts support relations between geometrical primitives and are thus more effective during the analysis. The topological geometries are arranged in hierarchies, i.e. a line is built using end points (generally called nodes) and additional supporting points (generally called vertices). A polygon consists of (surrounding) lines and a three dimensional volume of edges and polygons.

A detailed description of these data concepts is given in GRÖGER & KOLBE (2005) and WU ET AL. (2005). Diverse standards in the line of the ISO 19100, developed primarily by the Open Geospatial Consortium (OGC), can be consulted as a system of rules for the definition of primitives in geometrical concepts. The Geography Markup Language (GML, for 3D objects defined from version 3 on) was proposed by the OGC for data exchange. The implementation is oriented to the Internet's standard Extensible Markup Language (XML). The realization of these standards is occurring very slowly, even with the tools of the OGC members. This leads to data handling in rasters or triangles (TINs, Triangular Irregular Networks), which describe the enclosing surfaces or interfaces, however, better data concepts could enhance the modeling (see chapter 3.1.3). The spatial operations described in THOMSEN (2005) are used in wide areas and are feasible for geometrical as well as for topological objects.

In numerical modeling systems (e.g. soil water models, models of the unsaturated zone, and numerical groundwater models), there is no need for geometrical and topological concepts. The discrete elements are handled as cubes or prisms.

The database in spatial modeling is assessed also by geostatistical methods. The variogramm allows for determination of the support range. It can be calculated, according to BLÖSCHL (1996), as one-third of the range of the variogram model. On a more general level, the total range can be taken as well. Therefore, variograms should be calculated for each layer, horizontal and vertical, so that the minimal volume to be considered is determined statistically from a multiplication of the support ranges.

Structures that are smaller than the geometrical or topological volumes cannot be resolved by rasters or irregular triangles, of course. In contrast, the discretization by rectangles or triangles must be at least two times the resolution of the size of the smallest units that need to be considered. The realization in a GRID (rectangled or squared raster, cubes in 3D) or TIN (irregular triangles, prisms in 3D) leads to different views, but if the appropriate resolution is applied, the differences between both discretization methods can be neglected. The possibility of an automated adaptation of the discretization to the given data and to the structures that need to be represented exists in the form of so-called quadtrees, but modeling tools do not support this feature in most cases.

Several factors are important for the spatial discretization. First, the modeling task – and depending on this, the chosen modeling system – must be considered. The geological units and the hydrological and hydrogeological settings define the model resolution and outline in the second line. The representative elementary volume can only help to define the discretization and the total volume of the model in a few cases. Numerical models must satisfy additional conditions such as the Neumann criterion or the Péclet number for numerical solvers in flow and transport models.

Modern methods (e.g. those based on Voronoi or Thiessen polygons) allow for a resolution if there is a discrepancy between input and confidence intervals of the results.

Similar to the necessity of considering scale aspects in spatial modelling, the temporal discretization in dynamical modeling is of major importance. Often, the model purposes are defined predictively. This poses the problem of defining scenarios for the boundary conditions and parameters of the numerical models. BLÖSCHL (1996) shows some of the problems that arise in this process in detail. Difficulties in determining and defining anisotropies and enlargements of the model area are two of the most serious and most widespread mistakes in these scenarios, and they can arise even in the setup of successfully calibrated models. The models discussed here, with their high spatial discretization, should present fewer problems than do the spatially highly integrating dynamical models in hydrology, e.g. statistical precipitation and runoff models.

As with the spatial scale, the temporal scales of hydrological processes are most appropriate for the definition of temporal scales in hydrogeology. Temporal and spatial scales are connected and coupled in processes that can be observed and modeled.

BRONSTERT ET AL. (2005) define the following temporal scales for hydrology:

- Events that last for several minutes up to one day are called short-term events. They are very important in hydrology especially for the sizing of sewage systems and drainage systems. Flooding events sometimes fall into this class.
- Seasonal periods with a length of several days up to one year are called medium-term events. This time scale is most important in hydrogeology because several anthropogenic influences on water budgets have this periodicity, e.g. groundwater extraction for water supply or for irrigation. However, natural processes such as groundwater recharge also follow these cycles. Even the passage of cyclones and low- or high-pressure areas may cause cycles of a few days.
- The importance of long-term events with time horizons of several years to about 100 years has been increasing in recent decades. This holds true for hydrological as well as for hydrogeological models. Some examples are the calculation of the annual characteristics of hydrological events (e.g. floods or droughts) or of flow and transport processes in groundwater.
- Until recent times, longer time scales were rarely considered in hydrology. Only the research of climatic phenomena involves for such long periods. In hydrogeology, the interface to geological processes is more obvious. These processes were

of great influence to large catchment areas and aquifer systems. In some areas, this influence has persisted up to the present day. This will be shown in one of the case studies. In addition to the scales of BRONSTERT ET AL. (2005) historical scales (about 1000 years) and geological scales (about 1 mill. years) are defined. The climatologically and geologically important glacial periods are natural boundaries for these two scales.

In Figure 12 the time scales for the considered models are shown simplified in the form of a time bar.

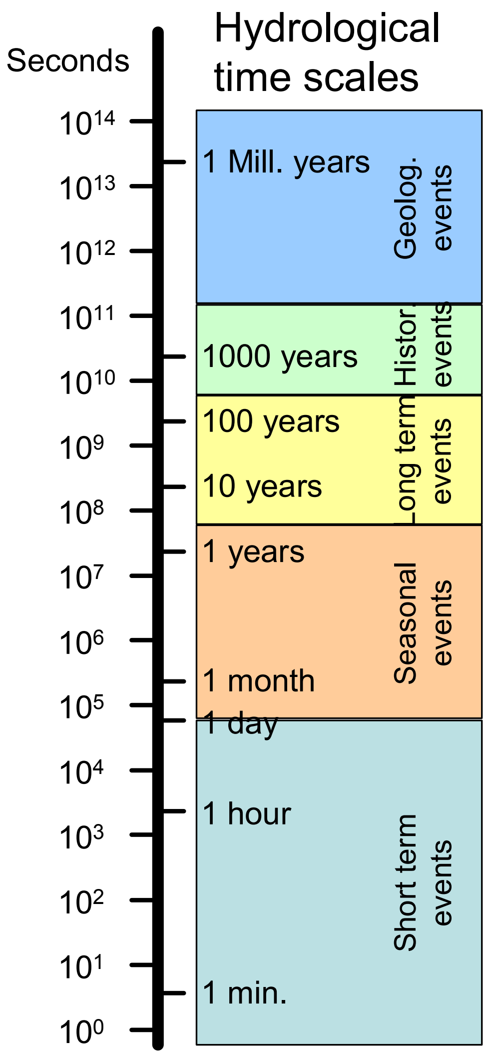


Figure 12: Time scales for hydrological and hydrogeological modeling approaches (adapted from BRONSTERT ET AL. 2005).

A differentiation of process-, sampling- and model scales is as necessary in time scaling as it is in spatial scaling. The process scale dominates the other scales.

BLÖSCHL (1996) describes the connection between temporal scales and spatial scales in hydrology. Based on the influence of geological processes on hydrogeological processes an upgrade to Figure 13 became necessary. The discontinuities between the scales of the different compartments are obvious – i.e. processes in the atmosphere, at the surface, and in the unsaturated zone, flow and transport processes in the saturated zone, and geological processes. Of course, there are evident intersections, e.g. volcanoes, earthquakes, and submarine slides, but most of the processes can be classified into the proposed scales.

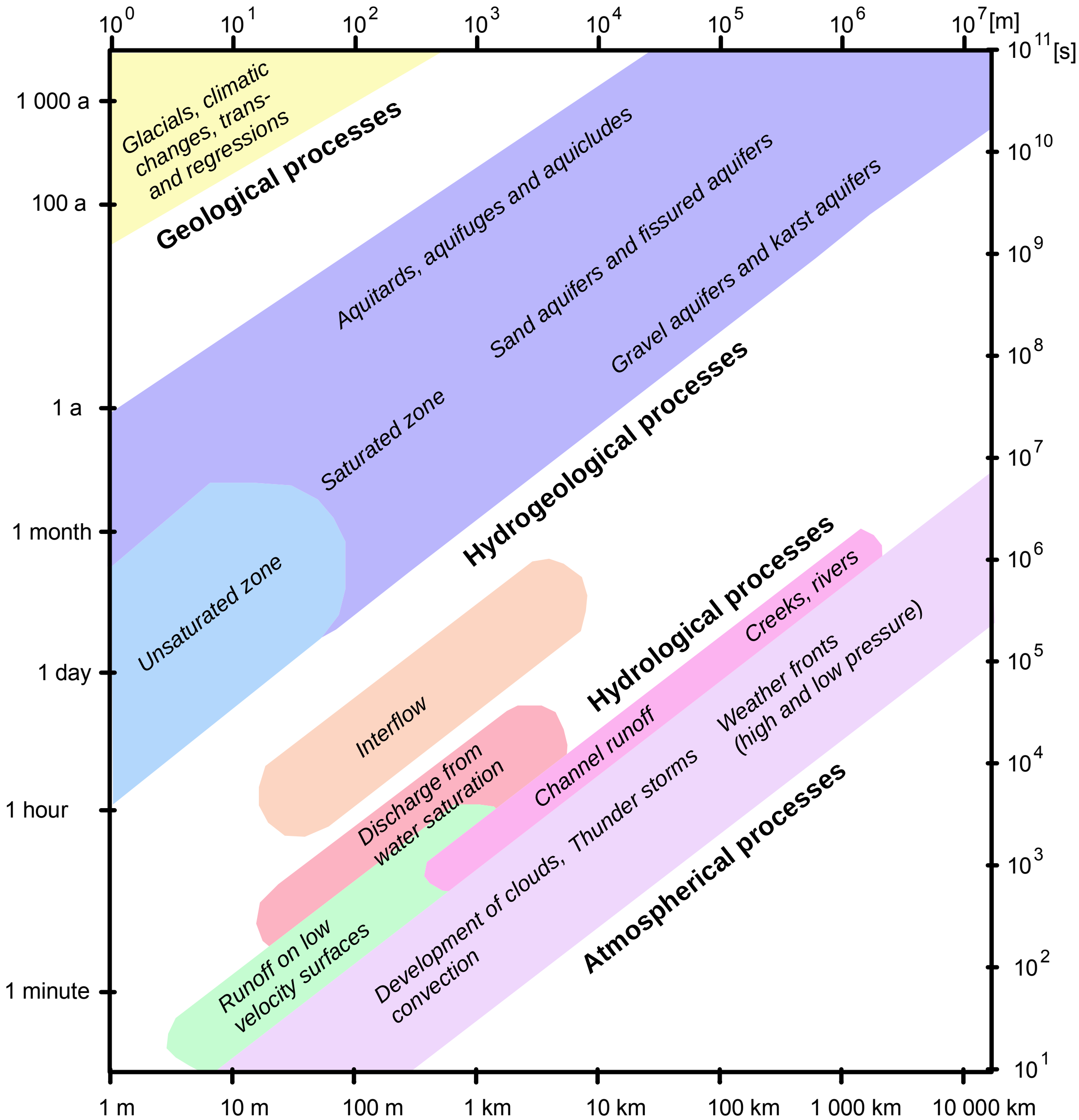
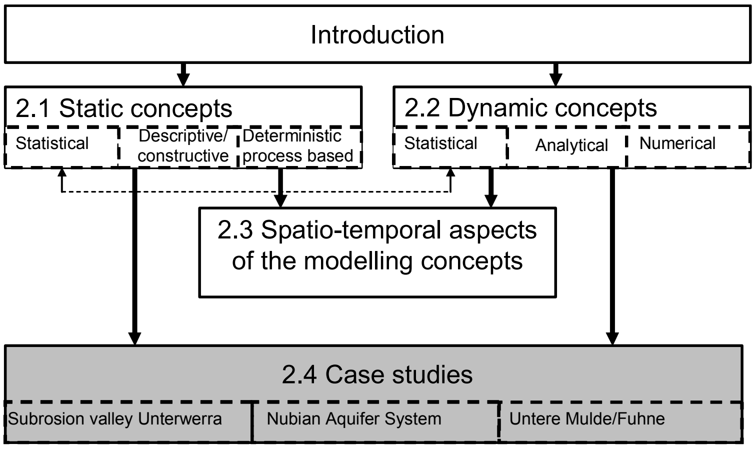


Figure 13: Connections of spatial and temporal process scales in hydrology and hydrogeology (adapted fromo BLÖSCHL 1996). Only flow processes are considered but no solutions or particle transport.

2.4 Modeling concepts of the case studies



All of the case studies introduced in chapter 1.3 were developed with static and dynamical methodical concepts. Various research topics are handled with these instruments.

In the first step, geological models on a static base were developed. Statistical and constructive methods were used for these models.

On these fundamental geological models, numerical groundwater models were built, so that the dynamical elements were added after the setting of boundary conditions and groundwater recharge. Furthermore, more models were developed for the step that enhanced the database for the numerical groundwater model. Only the model for Untere Mulde/Fuhne was reworked in a second step. From 1840 to 1990, the geological layers were disturbed by mining activities in a comparably short time span. An enlargement of the model area and additional geological modeling was therefore necessary.

2.4.1 Subrosion Valley Unterwerra

In the investigation area of the Subrosion Valley Unterwerra, many wells are used for groundwater observation. The sampling is carried out in periods of about six months and the measurements include hydrodynamical parameters as well as hydrochemical parameters. This excellent database for model setup and calibration leads to specific modeling concepts, which allow a pure statistical analysis for several hydrogeological questions. A static geological model was generated with constructive methods. Geological volumes were modelled for this geological model. LÄHNE ET AL. (2006) show that these methods are also suitable in this case, although the model area consists partially of hard rocks and partially of fluviatile deposits (e.g. gravel) and flooding sediments (clay and silt). Only a few specific features of the geology – i.e. remains of volcanoes and larger faults – were difficult to handle, but these problems were also solved.

The static geological model was used as the base for the hydrogeological numerical modeling. The dynamical elements in this case study were groundwater recharge and boundary conditions. The geological volumes were discretized into prisms for better handling and to facilitate numerical solution.

The characteristic feature of the model of the Subrosion Valley Unterwerra is the application of analytical methods in parameter determination for the numerical groundwater model. Aquifer tests, slug&bail tests and infiltration tests/open-end tests were carried out in a high spatial resolution. This fulfilled the need for a differentiated database for various hydrogeological and environmental geological research projects. In addition to the groundwater flow modeling models for groundwater vulnerability or aquifer sensitivity can be calculated on a high-resolution parameter set. Hydraulic conductivities were measured in the laboratory even for the hard rocks with adequate sample cores drilled horizontally into the unweathered material.

2.4.2 Nubian Aquifer System

Several research topics were focused on the numerical groundwater model of the Nubian Aquifer System.

- The socioeconomic conditions in Egypt and in the neighboring states of Libya, Chad, and Sudan make an extension of the water supply essential for survival. Programs for increased food production and drinking water supply fed by groundwater from the Nubian Aquifer System, have already been worked out for several oases in the Western Desert of Egypt, the eastern parts of Libya, and the northern Sudan. A numerical groundwater model with an increased resolution in the development areas should point out the consequences of simultaneously increasing groundwater extraction in different parts of the aquifer. Possible solutions to the problems should also be proposed.
- Prehistoric and geologic investigations in the Eastern Sahara revealed a wide distribution of surface water as indicated by the existence of limnological and fluviatile sediments and by archaeological discoveries. The reconstruction of large climatic changes was supported by further investigations in recent years. A better knowledge of the exchange of surface water and groundwater should be gained through the use of an extensive and long-term model. The genesis of limnic sediments, Sabkhas and paleontological findings (bones of hippopotamuses, crocodiles and large fish described in PACHUR ET AL. 1990) were also studied.
- The saltwater-freshwater interface in the North of the investigation area is subject to a most recent research project. The reasons of the wide ingression of saltwater are investigated based on the background of climatic changes in the last 140000 years.

The Nubian Aquifer System is surrounded by basement outcrops in the east, south, and west that perfectly fulfill the demands of boundary conditions. Two possibilities are given for a closing boundary condition in the north: in the models of BRINKMANN & HEINL (1986), EBRAHEEM ET AL. (2002), EBRAHEEM ET AL. (2003), EBRAHEEM ET AL. (2004), GOSSEL ET AL. (2004) and GOSSEL ET AL. (2006) the saltwater-freshwater interface is used as a no-flow boundary condition that reportedly has been stable for a few decades. In the further development of GOSSEL ET AL. (2004) and GOSSEL ET AL. (2006), the model was extended to the Mediterranean Sea and to the northwest of the area of the Great Sirte Basin (GOSSEL ET AL. 2010A). A boundary condition was used in this model that was much more reliable than the saltwater-freshwater interface, which was observed only over a short time compared to the general flow velocities.

The database of the Nubian Aquifer System is completely different from the database of the Subrosion Valley Unterwerra. Hydrogeological parameter tests are very rare, and they are only scarcely available in the literature. The situation for geological understanding and modeling is slightly better owing to a Special Research Programme of the German Research Foundation during the 1980s and 1990s. The primary dataset from drilling reports, aquifer tests, and water level measurements is only adequate for the oases that were studied by the first hydrogeological investigations mentioned above. The hydrogeological structure and the parameters for the model of the Nubian Aquifer System were developed by a mixture of constructive and statistical methods. The modeling of geometrical or topological volumes was not adequate for the extension and purpose of the numerical groundwater model. Therefore, only discrete elements were modeled.

The geological and hydrogeological basics of the model were described in detail in GOSSEL ET AL. (2004). In the central parts of the model area the database consists of cross sections and single borehole data of deep wells with an analysis of aquifer parameters. Thus, the database is assumed to be sufficient for such a large and long-term model. At the edges of the model area, the geological database is nearly insufficient, and it can only be completed by geostatistical methods in the sense of an extrapolation. For the research projects outlined above, different numerical groundwater models were created. The long-term models are finite element models that are discretized relatively evenly in horizontal dimensions. In the coastal region only, the resolution was enhanced owing to the proposed effects of saltwater intrusion (GOSSEL ET AL. 2010A). The model for the investigation of the recent and supposed future groundwater extraction was highly discretized for the oases, where the effects had to be investigated in detail (SEFELNASR 2007). Additionally, a detailed model of the coastal area was developed with a very high vertical resolution and with the horizontal resolution of the model described in GOSSEL ET AL. (2010A).

All the modeling tasks with their high divergence in temporal and spatial resolution were carried out with dynamical numerical methods and were based in principle on the same static geological model that was built through a mixture of constructive and statistical methods.

2.4.3 Untere Mulde/Fuhne

For the area Untere Mulde/Fuhne static models were developed for the following tasks and objectives:

- Multivariate analysis and ranking of pollutants (THIEKEN 2001).
- High spatial resolution geological modeling (FABRITIUS (2002) and WOLLMANN (2004)).
- Assessment of distributions of contaminants.

According to the highly diverse tasks, the investigation areas were changed for each model. The statistical analyses are bound only to the modeling task and the availability of data for defining the outline of the area. The geological model, which in the first phase was built by FABRITIUS (2002), was enlarged according to the observed structures by WOLLMANN (2004). The hydrogeological model, which is fundamental for the reported research, is oriented to the hydrological and subordinated geological conditions.

THIEKEN (2001) identified the most important substances from the large pool of hydrochemical analyses of the monitoring program carried out by the federal state of Saxony-Anhalt. The statistical methods included factor analysis and the Hasse diagram technique (BRÜGGEMANN ET AL. 1999). The substances are considered to be most significant for further sampling, analyses, and observations, as well as for the analysis of the already-gathered samples and for future monitoring strategies. Additionally, regional and geological genetic characteristics were used for the identification of spatial signatures.

In other reports, two- and three-dimensional distributions of hydrochemical parameters were calculated (RICHTER ET AL. 2004, WYCISK ET AL. 2004a, WYCSIK ET AL. 2004b) with geostatistical methods. RICHTER (2003) used additional information such as the geothermal gradient and conceptual models of hydrochemical reactions for his analyses. In WYCSIK ET AL. (2004b), the analysis of significance was the focus. This topic was important because of the spatially highly heterogeneous sampling in the past. In addition to the pure geostatistical analysis, the investigations had been accompanied by a first numerical groundwater modeling attempt worked out by NEEF (2002) for a rather small investigation area. This modeling approach was proven to be insufficient, thus, it was enlarged to a regional scale so that the contamination sources, mining areas, and reliable boundary conditions became part of the model area.

In addition to the statistical models, high-resolution geological models were created for the central area of the contamination at the Bitterfeld megasite because the environmental models were not intended to explain all observations. The geological models helped to determine the reasons for the distributions of hydrochemical parameters in a more detailed way. FABRITIUS (2002) generated a model of the southern part of the area, which since 1975 has been affected by open pit lignite mining and the subsequent rising groundwater levels. WOLLMANN (2004) constructed the model for the northern part of the area. Here, the effects of the rising groundwater following a large flooding event in August 2002 in relation to the spread of contaminants were very important. In WYCSIK ET AL. (2006), the geological and hydrogeological investigations in this area were connected and interrelated.

For the geological modeling a geometrical concept was applied in the first step. A discretized version of this geological model was then built by the modeling system.

Although the tasks, modeling systems, methods and tools were very diverse up to this point, they served for the development of a complex assessment of the contamination in this region with high heterogeneity in geology, mining, and industrial history.

Considering the geological models developed by FABRITIUS (2002) and WOLLMANN (2004), which covered a total area of about 60 km² a regional numerical groundwater flow model with an area of about 320 km² was generated. This model had to be constructed on the concept of discrete volumes. A realization by geometrical volumes was not applicable in this model size, and it was not necessary for the model's purpose to continue with this concept. The use of statistical methods was essential for all kinds of model setups for the areas outside of the areas of the detailed geological models. The temporal dimensioning of the numerical groundwater model demonstrates the necessity of considering dynamical components: the model does not focus on flow regimes with a high spatial resolution or the distribution and spreading of contaminants. Even the assessment of anthropogenic impacts as the remediation activities is neglected. The main topics are the investigation of regional flow systems that depend on regional geological features and the development of these flow patterns over an extended time span. The mining activities in the last 150 years with rapidly changing spatial impacts and pollutions from the chemical industry occurring for over 100 years have led to a very complex and challenging modeling task, in geology as well as in hydrogeology. The geological structure was changed completely over large parts of the area by the open pit mining. This digging and dumping of material (including wastes) occurred dynamically, travelling all around the town of Bitterfeld. An overview of this is shown in in Figure 14.

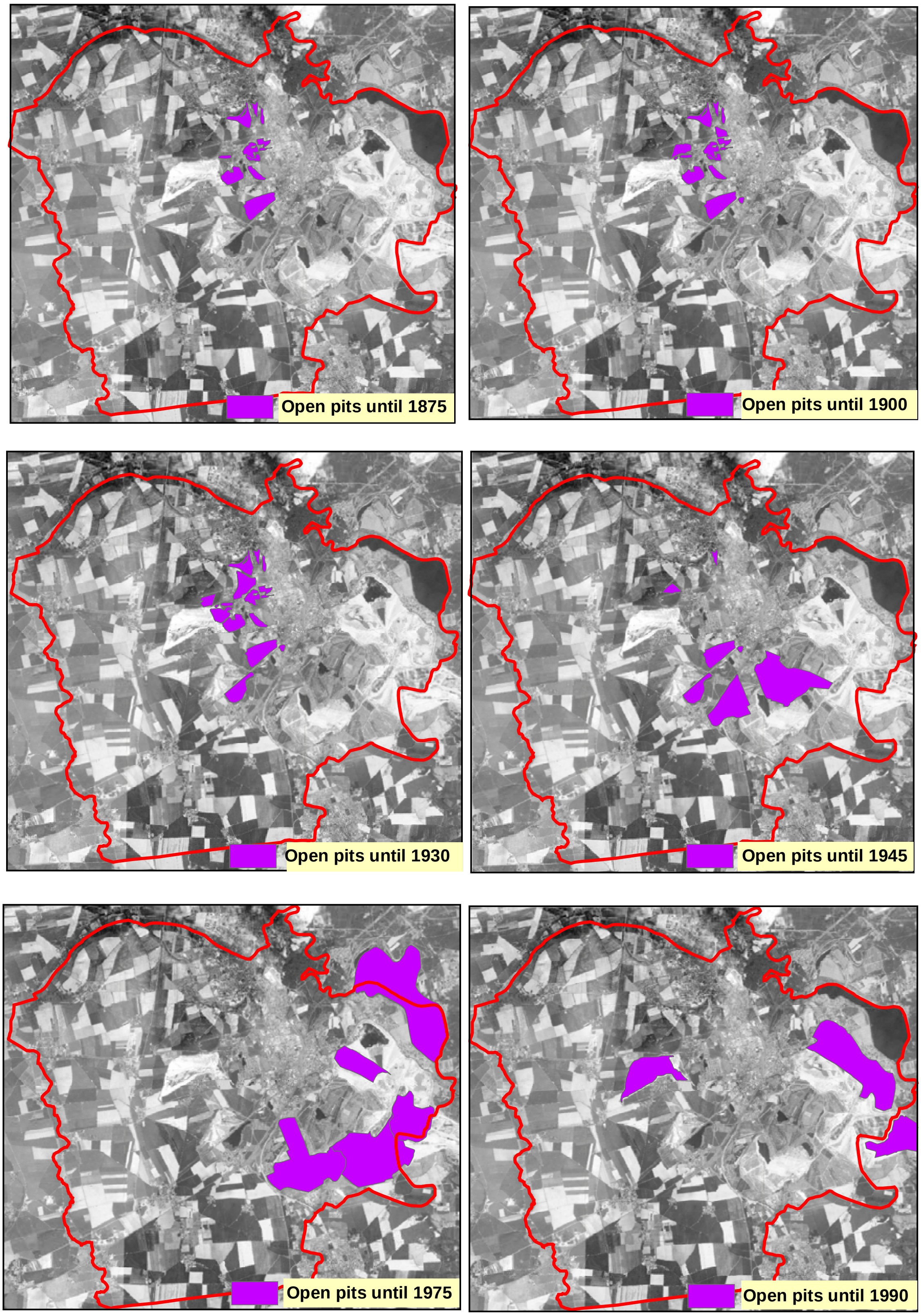


Figure 14: Dynamical development of the lignite mining in the region of Bitterfeld. The various time slices show the traveling directions of the areas to the west of the town via the south to the east. This causes changes in the overburden and the mine dumps. The mining depth is thus also influenced.

2.5 Summary of modeling concepts

The modeling concepts can be grouped into static and dynamic concepts according to their time dependency. The derived models rely on these concepts. Both modeling concepts work with different methods. Their application is directly tied to the purpose of the model. The availability of data should influence the choice of a modeling concept only in the second line. The different applicabilities and applications of modeling methods and modeling systems have changed over time. Today, statistical and descriptive methods are dominant for the static concepts, while numerical methods are preferred for the dynamic concepts. The described concepts are fundamental and therefore, it is possible within the aspect of the two main concepts to classify the coupling and the interfaces of modeling systems using a systematic approach. In the case studies of Untere Mulde/Fuhne, the Nubian Aquifer System, and the Subrosion Valley Unterwerra different concepts were applied, and the methods employed were briefly described.

3 Modeling systems

The generation of a conceptual model is fundamental to modeling. This task can be carried out with knowledge of complex modeling systems as provided in this report. This knowledge about the development of a conceptual model through methodical and systematic solutions is as vital as additional data that will be incorporated into the model. These developments depend on each other.

The modeling systems that can be used for this task must fulfill one of the concepts described in chapter 2.1 and 2.2. The technical solutions are reduced in most cases to either static (spatial or temporal) or dynamic modeling concepts. In a certain way, modeling the steady state is a transition from static to dynamic concepts. In steady state models, the methods of dynamic concepts are used to focus on a quasi-static equilibrium, e.g. in chemical reactions or in groundwater flow. For the coupling of modeling systems as described in chapter 4, it becomes necessary to go beyond this difference, at least for the data exchange.

This chapter focuses in detail on the modeling systems and therefore on the realizations of the concepts according to the applicable or available methods. The task will not be a description of computer models or the possibilities of connections of modeling systems, as discussed in chapter 4. There will be no comparison of modeling systems – they are in continuous development, and any comparison will be to some extent outdated. In chapter 3.8.4, only the modeling tools for the case studies are mentioned as examples. Figure 15 provides a graphical overview of the chapter.

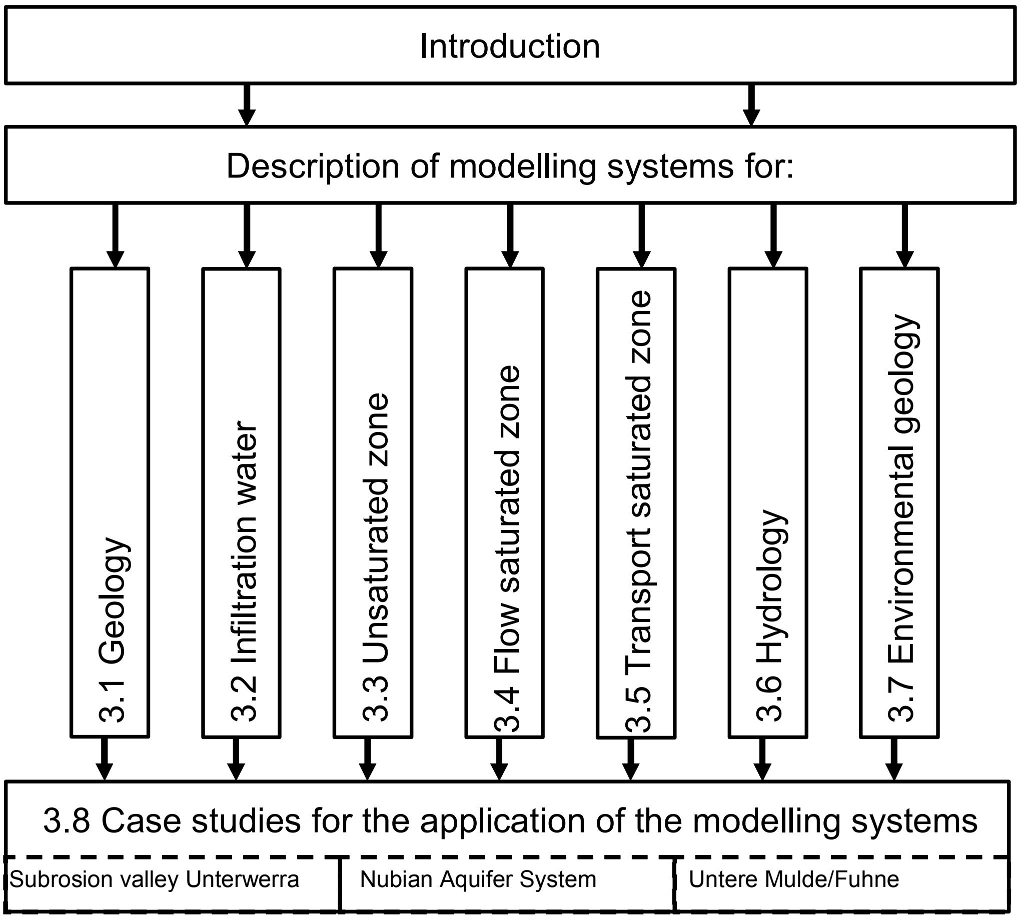
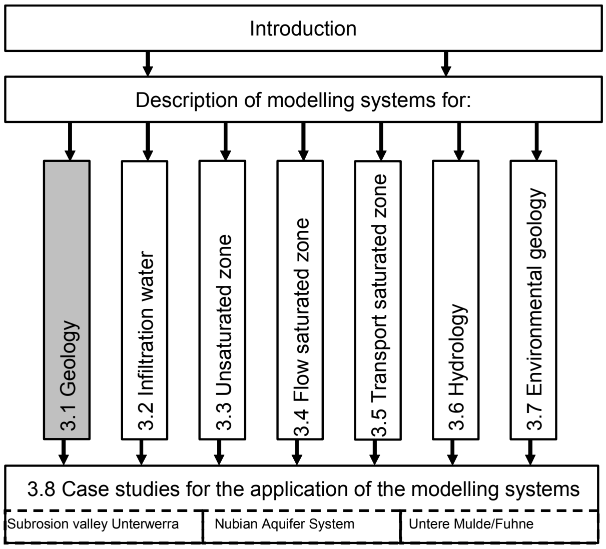


Figure 15: Graphical overview of chapter 3. For better orientation, this graphic is set as a miniature at the beginning of each subchapter.

3.1 Geological modeling systems



Geological models are needed beneath the pure geological interpretation for further analysis. One aspect is environmental geology, as described in WYCISK ET AL. (2002). The estimation of residual contaminations in sorption horizons or secondary sources of contamination, where the contaminants are gathered in depressions of aquifuges and are only slowly resolved, are new applications in environmental geology. A topic more related to hydrogeology is the finding of hydraulic windows, i.e., connections between aquifers or gaps in aquicludes that may lead to an exchange of contaminants between two aquifers.

Geological modeling systems use static modeling concepts in most cases. Dynamical elements play a role only in long-term models or in studying anthropogenic effects, such as those caused by open pit mining. The development of dynamical geological models is complicated owing to this narrow field of possible applications and thus it is bound to the development of new concepts.

In the hydrogeological context, static geological models are used mostly for the supply of structures and parameter distributions in numerical groundwater models. In tools used for numerical groundwater modeling, the geological modelling tools are therefore often implemented as pre-processors. The step from the geological model to the numerical groundwater model is much more complex than what is anticipated based on the integration in the tools:

- The parameter distributions of numerical groundwater models (e.g. hydraulic conductivities, storage coefficients, sorption coefficients) are not directly connected to the geological model, because geological models are mostly stratigraphically classified.
- The numerical algorithms place demands on the model structures that have nothing to do with geology and that are thus difficult to satisfy with complex geological models.
- The effects of an excessive simplification of structures and parameter distributions may be very serious and may lead to incorrect assumptions.

A deeper consideration of this modeling concept must go far beyond the statistical generation of distributions.

CHRISTAKOS ET AL. (2001) showed, based on historical information, that geological models are not suitable for predictive or prognostic calculations. Geological modeling systems are advantageous primarily in relation to descriptive models.

Geological processes are easy to describe literally. However, these descriptions are not mathematically formulated and thus are not applicable (or only minimally applicable) to computer sciences. The difficulty of modeling geological processes is bound, to a certain extent, to the lack of measurable input data. In most cases, geological processes can only be identified according to their results (a posteriori). Thus, geological process models must rely on inverse modeling. Furthermore, many processes cannot be modeled according to direct results inversely, because only proxy data are available for these processes. A few steps towards geological process modeling are presented in GALLOWAY & HOBDAY (1996).

Figure 16 presents the general procedure of geological modeling. It starts with the field data and additional knowledge and moves up to the results that can be used for almost all objectives in geology. For the most part, the digital data acquisition is already integrated in field investigations. This simplifies the following steps of interpretation and modeling.

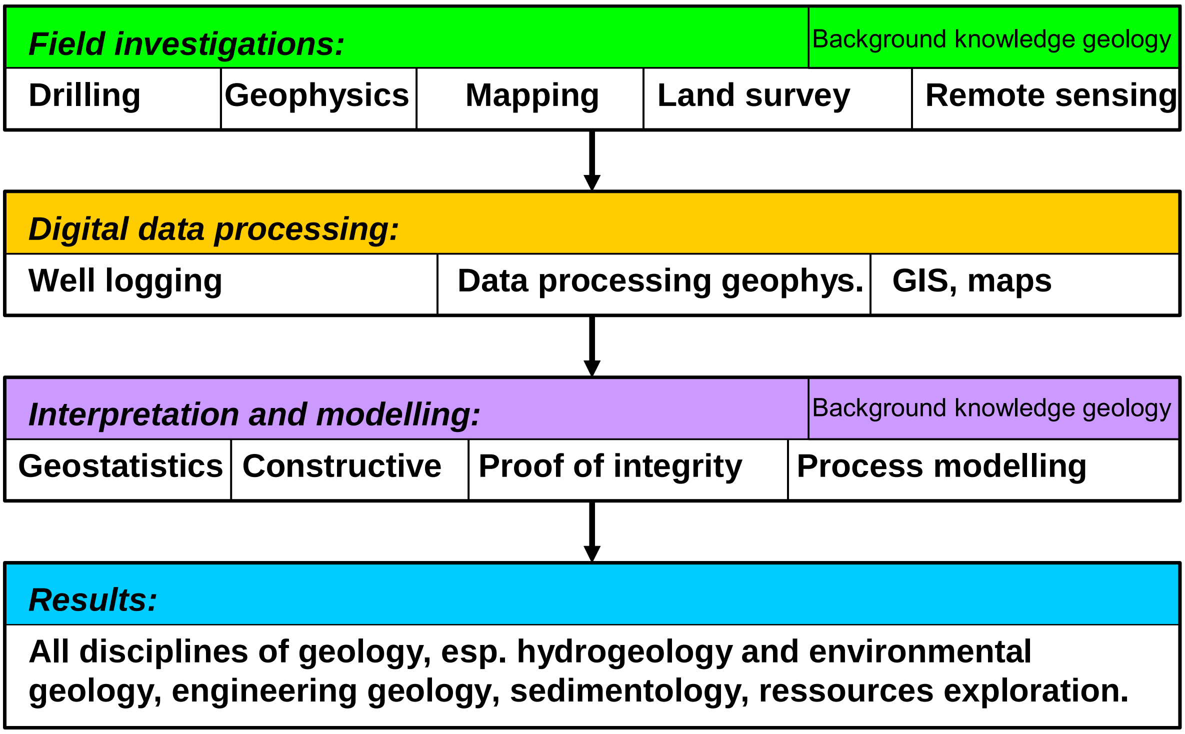


Figure 16: Geological modeling. The procedure of building a geological model can be made much more efficient by using digital means that are already present in the field. Geostatistical, constructive, and process-based methods are not used alternatively but integrative in an increasing number of applications.

3.1.1 Input data for geological modeling systems

The heterogeneity in geological databases used for geological modeling was described in detail by HOULDING (1994). Therefore, only a few special aspects of the very diverse database need to be emphasized:

- In contrast to a very low sampling rate in horizontal dimensions, the vertical analyses of borehole data are very dense.
- The database for modeling tasks in hydrogeology and environmental geology are not feasible in a regular raster, as in economic geology or mining.
- The database of boreholes can be improved only in the long term and with intensive technical efforts.

- Geophysical data – e.g. geoelectrical investigations, seismic profiles, or complete 3D seismic profiles – are not available for most projects in hydrogeology and environmental geology, and thus they are rarely applicable. Additional problems arise from the excessive effort involved in interpreting the gathered data and from the need to reduce the data to distinct tasks and geological conditions.
- Adjacent to the borehole data with high vertical resolution and low horizontal resolution are the geological map and a DEM with high horizontal resolution that is reduced at the surface.

This framework shows that it is vital for these modeling systems to have the capability of importing additional data on account of the heterogeneous database. Nearly all data are welcome, but they need to be qualified and this qualification of the data origin must be taken into consideration in the modeling system and the modeling process. The borehole data are often not classified stratigraphically or lithologically correct and thus are not easy to interpret. Also, a knowledge based completion of datasets based on a constructive or statistical method, must be transparent. This procedure should also be easy to correct in case some interpretation proves to be wrong during the modeling process. The modeling tools should be able to differentiate between the following diverse levels of data security and data quality:

- safe data,
- data with an uncertain geological classification,
- additional data from secondary data sources and investigations, i.e. geophysical data,
- proxy data,
- constructive enhancements of the database,
- statistical enhancements of the database.

These levels of data quality have nothing to do with the support range calculated by geostatistical methods.

Additional formal uncertainties arise if classified data, instead of continuous data from secondary data sources, are used for modeling.

Boreholes as input data for modeling have the advantage of an at least lithologically definite systematic classification (if a core is investigated). Nevertheless, these data are spatially restricted to a local scale because their support range is very short. For the density of borehole data in Germany, an overall value of about 1 borehole per km² is realistic, as has been documented for regional geological models. A borehole depth > 10 m is necessary for hydrogeological modeling (SOBISCH 2000 and GOSSEL ET AL. 1998). In mining areas, this number increases considerably; in hard rock areas the density in wide areas is much lower than the overall value. Thus, many large data gaps can be filled by geophysical data. For geological modeling with a heterogeneous database, WU ET AL. (2005) propose interesting and important methods.

Geological maps as additional data sources for geological modeling are absolutely necessary because they provide rare information about the horizontal distribution of geological layers. The importance of geological maps is often underestimated by geological modeling tools because most of them focus only on deeper reaching information.

The outline of geological models is, in a first attempt, only bound to the model's purpose. The reduction of geological volumes is normally possible in all modeling tools without any problems. The outlines of geological boundaries should be preferred for the outline of the model area. For modeling with discrete elements, a resolution or discretization should be oriented at the smallest geological volumes; otherwise, these volumes cannot be mapped in an appropriate way.

3.1.2 Modeling methods

Statistical modeling systems have been enhanced by advances in geostatistical analysis and interpolation methods. These methods were applied successfully to many geological research projects. In the beginning, there were the very important economic estimation and investigation of mineral resources, but now these methods are also applied in general geology, especially for the generation of structures (MALLET 2002). Different kriging variants were described by DAVIS (1986), AKIN & SIEMENS (1988), ENGLUND & SPARKS (1988), ISAAKS & SRIVASTAVA (1989), DEUTSCH & JOURNEL (1992), HEINRICH (1992) and SCHAFMEISTER (1998). For scientific questions, other (geo)statistical methods – such as conditional simulation (SCHAFMEISTER-SPIERLING 1990), simulated annealing (DEUTSCH & JOURNEL 1992), and genetic algorithms – were developed and applied to diverse projects.

The implementation of constructive methods in geological modeling systems is not often documented in case studies. SOBISCH (2000) describes the development of a three dimensional geological model of the map area of Nordhorn (Lower Saxony). FABRITIUS (2002) and WOLLMANN (2004) describe the use of constructive methods for modeling two areas around Bitterfeld. POHLERT ET AL. (2004) use constructive methods for a small model area in Leuna (Saxony-Anhalt), SCHLESIER (2006) and POHLERT ET AL. (2006) for the urban area of Halle (Saale), and LÄHNE ET AL. (2006) for the Subrosion Valley Unterwerra.

Process-based methods are rarely applied to geological modeling. In oil exploration, sedimentological modeling systems are used sometimes employed. The methods are restricted mainly to classical sedimentology in litoral and fluviatile environments. In addition, in the study of tectonics, modeling systems are applied for interpretation, but these rarely have a process-oriented character.

For the geological handling of input data, scientific geological knowledge is very important. As shown in chapter 2 geological settings – e.g. the outline of former coastlines, the distribution of faults and fissures, glacial channels, and gully erosion systems – have to be taken into consideration. Although borehole data and measurements have the highest priority, these knowledge-based data are vital for a good interpretation. This background knowledge can be applied more readily to constructive methods than to statistical methods, because in geostatistics the only way of influencing the interpretation involves the variogrammetry. In constructive methods, the visual modeling techniques depend on the integration of this knowledge, which is already present in the visual modeling procedure.

Both methods have benefitted from the advances in computer sciences. Geostatistical methods require a great deal of computational power and good software algorithms. The constructive methods were improved by the development of visualization techniques. Three-dimensional images are important for the visualization and control of geological models built with constructive methods. Presently, the possibilities of interaction are only restricted when the model needs to be corrected or when new data become available.

Both kinds of modeling are needed in the modeling process. Normally, the statistical modeling techniques need additional information that is given via supporting points. These points may be derived from geological maps, geological knowledge about certain horizons, etc. The constructive methods depend on interpolation techniques to obtain a spatial distribution from the digitized cross sections.

Additionally, there are diverse problems for the modeling systems themselves in regards to the complete application of their concepts:

Most of the practical 3D applications have no ability to create, interpret, and implement different variograms for horizontal and vertical dimensions.

Constructive working methods experience a problem in which a very high data density is created along the cross sections, whereas in the areas between these cross sections the appropriate interpolation methods must be applied. Each interpolation, for either the top or the bottom of a geological layer, must be performed, so that the surfaces are resulting for the whole pile of layers existing in the total area. Erosive geological structures are thus identified and reproduced. For this method, the interactive work with high-speed interpolation and presentation of the layer tops or bottoms is essential in finding and eliminating mistakes as soon as possible. Therefore, in most tools, triangulations are the preferred interpolation method. If the triangulation is created automatically, e.g., by the Delaunay algorithm, geological structures often can not be expressed in a sophisticated way. Correcting this net of triangles manually produces better results. The application of geostatistical interpolation methods does not produce better models in most cases because the constructive modeling process already includes the interpretation of the data and therefore additional geostatistical interpretation is redundant. On the other hand, the geostatistical analysis of the data can be used as important information for other (modelling) purposes.

Statistical and constructive methods are implemented in several modeling tools to support their combination in the modeling process. The presence of both types of methods in modeling tools is so variable that the tools could be called hybrid tools.

3.1.3 Results of geological modeling

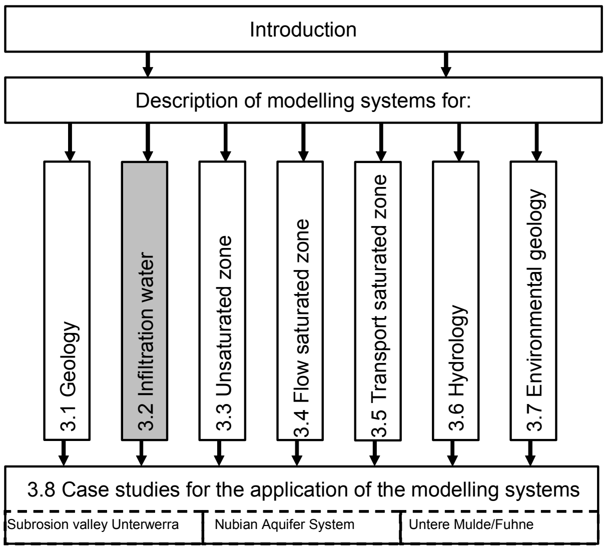
The result of the geological modeling is a stratigraphical, and sometimes also lithological or petrological, model of the layers in the subsurface. A differentiation between geological phases resulting from various sedimentation conditions or even continuous distributions between them, different mineralogical composition and biocenoses cannot be accounted for in these models. This leads to comparably high vertical inhomogeneities with suppressed horizontal inhomogeneities.

According to the modeling system for the geometries of the model, raster objects, geometrical volume objects, or topological volume objects are the results. The visualization possibilities are restricted to the availability in the modeling system. A feasible solution may be the use of standards in visualization that allow additional software, independent of the modeling tool itself, to include enhanced visualization capabilities. Exchange capabilities are also limited to a very small number of formats. For this purpose, the formats of the Virtual Reality Markup Language (VRML) or the Drawing Exchange Format (dxf) of CAD systems are usable. Another possibility arises from the pure visualization standard OpenGL. The description of the objects can be used by additional software to visualize 3D objects on 3D screens. These formats are suitable for the exchange of geometrical volume objects, though they are sometimes restricted in visualization related to spatial transformations. Topological formats are not generated and saved in most modeling systems, but the functionality and the topological operations are applied in the software tools of the geometrical data model.

The geological models are a very important basis for a first interpretation in hydrogeological modeling. The possibilities in hydrogeological, environmental geological and hydrological interpretation will be considered here. One possible result from geological modeling is the model-based outline of hydrogeological structures that can be studied without any further modeling, e.g. the structures of aquifers and aquitards or aquifuges. Potential horizons for interflow, traps, and thus secondary sources of contaminants can be identified. In connection with further research and lithological investigations, the volumes of potential sorption horizons and thus the sorption capacity of these layers can be estimated. Spatial distributions of connections between aquifers can be identified from the structure of aquifers and aquitards.

For exchange with other modeling systems, raster-based or voxel-based ASCII formats are provided preferably by the modeling tools. Therefore, it is often necessary to convert geometrical volume objects to discrete volumes. As with the problems in 2D (in GISs), different possibilities of representing volumes are potentially given. In practice, they are exclusively restricted to one method. Therefore, different models may result from a conversion according to the center or the total volume of a cell. A solution to these problems may involve increasing the resolution of the model.

3.2 Modeling systems for infiltration water



A modeling system for infiltration water describes the vertical flow and, in most cases, the transport of solvents in the soil, i.e., the uppermost 2 m of the earth's crust. The following distinct modeling methods must be recognized:

- Empirical modeling systems without a physical structural modeling, e.g. the modeling systems of GLUGLA & GOLF (1987), DÖRHÖFER & JOSOPAIT (1980), SCHROEDER & WYRWICH (1990), GROSSMANN (2006), and WESSOLEK ET AL. (2004). Empirical modeling systems are based on varying proportions of analytical and statistical methods. It is most important that all empirical modeling systems attempt to mirror, to varying extents, the systematic structure of the physical processes.
- Catchment reservoir or storage modeling systems, e.g. in PFÜTZNER ET AL. (1992), PFÜTZNER (1994), WESSOLEK (1989), and HÖRMANN (2005). Catchment reservoir or storage modeling systems are based on numerical solutions of the simplified physical processes. They also include varying parts of statistical solutions.
- Complex numerical solutions that are based completely on the modeling of the physical processes.

The input parameters of the modeling systems vary as much as the internal methods of the modeling systems.

Figure 17 shows the general procedure of modeling infiltration water. For the whole modeling process, the application of GIS is necessary, especially for spatial data preparation and for the visualization of the results. Very often, GIS is even used for modeling the process itself. For these tools, an implementation of the algorithms in a standard computer language is very important in regards to updates and further development.

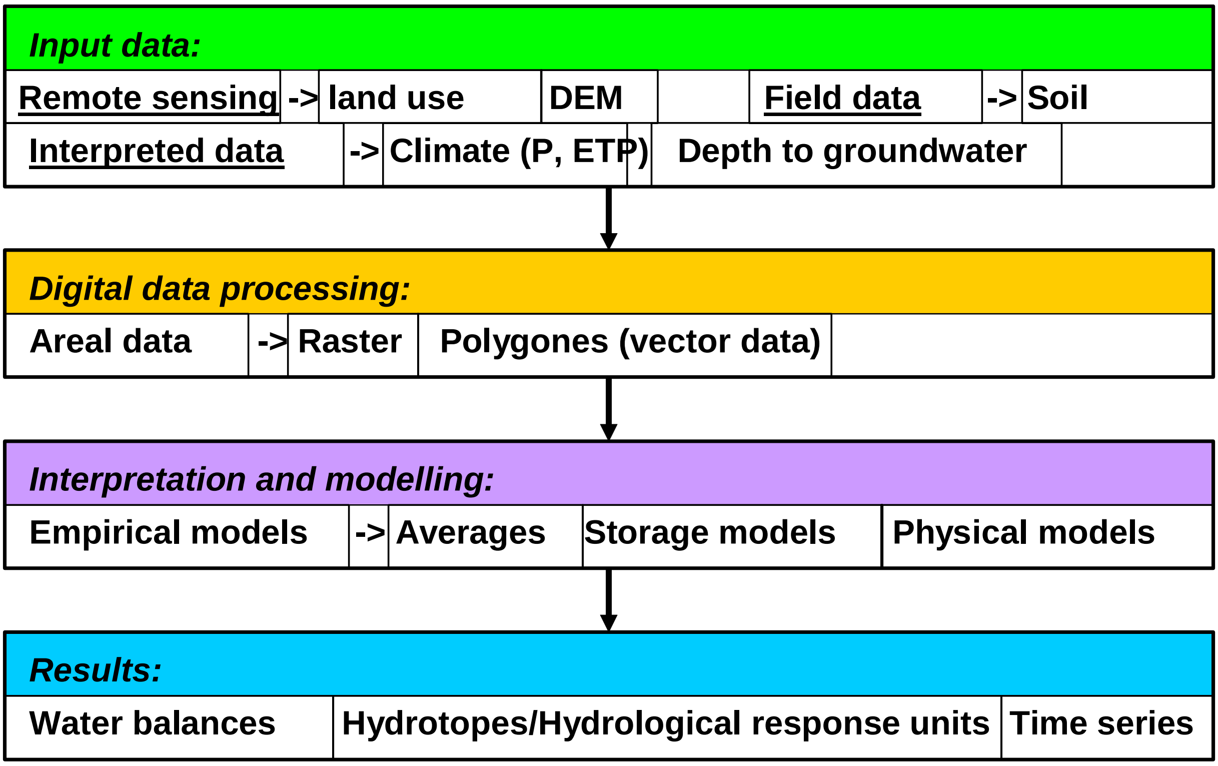


Figure 17: Infiltration water modeling. The input data are generally recorded digitally, but the data must be prepared in suitable form. (P = precipitation, ETP = potential evapotranspiration).

3.2.1 Input data of modeling systems for infiltration water

Input data for all modeling systems is climatic data, along with information about land use, soil, depth to groundwater, and sometimes the slope of the surface.

The climatic data are highly time dependent and include precipitation and evapotranspiration. Mostly, the potential evapotranspiration serves beneath the effective precipitation as an input parameter. Some modeling tools calculate this parameter internally from measurements of temperature, relative humidity, radiation balance, and/or wind velocity. In Germany, the appropriate methods are given by THORNTHWAITE (1948), HAUDE (1952), TURC (1961), and PENMAN (1948).

The other parameters are, in most cases, bound to two spatial dimensions. The available topographical maps and remote sensing data are used to derive parameters of the land use in terms of vegetation, development, and sealing. For the soils, the most important parameters are field capacity, permanent wilting point, hydraulic conductivity, capillary action, and sometimes even the suction pressure curve. At least an interpolation of groundwater levels must be used for the calculation of the depth to groundwater. The result of a (calibrated) numerical groundwater model is better, and those groundwater levels must be subtracted from the ground surface (DEM). The digital elevation model (DEM) is also needed to calculate the slope if this parameter is taken from a model for infiltration water. The DEM is very sensitive because it is used two times in the modeling process. It is very dependent on the scale.

All this data can be handled in a GIS method in two ways:

Vector-based methods require polygons, and they have the advantage of producing results of high spatial accuracy. This accuracy may be only an apparent accuracy on account of different scales and resolutions of input maps. The disadvantage of an intersection of different polygon data sources is the creation of sliver polygons, which are very small polygons that result from maps with different scales and databases. These sliver polygons must be aggregated after the intersection in a hydrologically consistent way.

The results of this intersection process are so-called elementary areas, which are aggregated to hydrological response units (HRUs) – in German “Hydrotope”. These hydrological response units are thus areas that have homogeneous and equivalent hydrological behavior (in this case, especially in regards to the infiltration water). The calculation of the infiltration rate needs to be carried out on these HRUs only after the process is complete.

On the one hand, the data handling of raster-based methods is very storage intensive. On the other hand, there will be no sliver polygons and thus no need to eliminate them. The possibility of data being aggregated to HRUs is also given in raster data handling.

The DEM, and therefore the input parameters of depth to groundwater and slope, are in most cases predefined as a raster dataset. They must be classified according to the hydrological criteria of the modeling system if they need to be intersected with the polygon data of soil and land use after the first processing (calculation of depth to groundwater and slope).

If the data for land use and soil are used from raster datasets, e.g., in the case of using remote sensing data, a raster data handling is clearl necessary. If some vector datasets need to be integrated into raster data processing, the conversion methods of a GIS can be used, but the conversion results should be analyzed in detail. Sometimes, an increased resolution must be chosen for all thematic data.

According to a mainly vertical orientation of the modeling approach, there are no bounding conditions for the horizontal extent of a modeling area. The discretization is bound on the one hand to the available data and on the other hand to the applied methods. A resolution of a 1 m raster is not useful, even in the case of a high-resolution input dataset, because the (mostly empirical) methods are not suitable for such a high resolution. The vertical extent of the model is also bound to the modeling methods. In most cases, the unsaturated soil with a thickness of 2 m is modeled. For the modeling of deeper layers, modeling systems for the unsaturated zone are used.

From the combination of time-dependent and spatially distributed datasets, a very complex data structure is received. In most cases this cannot be handled by a GIS in an effective way. Through a reduction of the time dependency to mean values or annual data for a few years, the infiltration rates or the groundwater recharge rates can be managed in the attribute database of a GIS.

3.2.2 Methods for the calculation of the infiltration rate

The selection of a suitable method depends essentially (beneath the modeling purpose) on the input parameters.

The empirical modeling systems can be parameterized via GIS methods in an easy way. These models have a short runtime. Owing to their pure empirical algorithms, these models are based on a low time dependency, though they are process oriented. Normally, the rates of average years are calculated based on average yearly sums or mean values, but annual values can also be calculated without serious complications. A higher temporal resolution requires the availability of an adequate time series of the land use parameters. In particular, the growth of crops must be considered in an interannual – i.e. monthly or daily resolution – modeling approach. One method that does not take the growth of plants into consideration is described in GOSSEL & WYCISK (2006). Thus, the results of this method are only an estimation of the actual infiltration rates.

Storage modeling systems work with a discretization into “compartments”, i.e. layers that can be represented by storage parameters. Via the water balances of the main components of the water cycle, the exchange of infiltration water, capillary rise, water saturation, and filling of the storage are calculated. The consideration of land use, the depth to groundwater, and the slope is nearly the same as in empirical models and thus are very application oriented. The input parameters are comparable. The advantage of these modeling systems is their high temporal resolution. In contrast to the empirical modeling systems, monthly or daily infiltration rates can be calculated according to the integration of time varying land use parameters, if necessary. The soil parameters are also discretized in a manner that is different from what is used in empirical models. In storage modeling systems, differentiation of the soil into several “layers” is possible. The modeling systems are normally not very sensitive to variation of the parameters in deeper layers. In most cases the sensitivity analysis of the modeling systems shows no significant differences between the results of models with a high vertical resolution and the results of those with a hydrologically meaningful aggregated small number of layers. Thus, the higher discretization only makes sense if the integration of the data from the geological model is seamlessly achieved using computing methods.

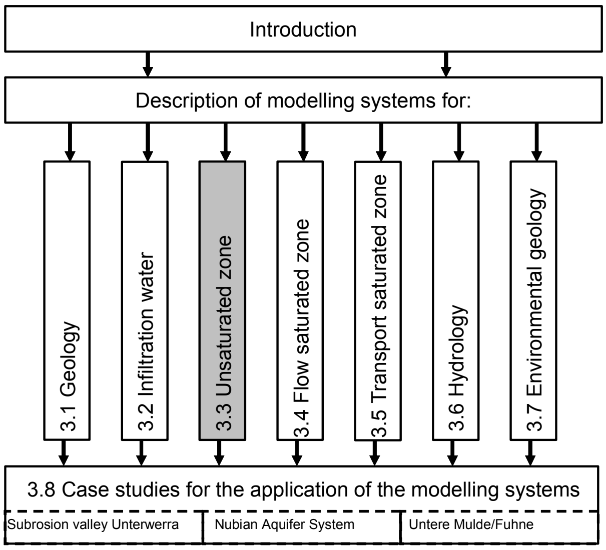
The numerical modeling systems that are based on the physical laws depend on a number of input parameters that are very difficult to obtain or to derive from available datasets. Some examples are the resistance of the stomata of plants and actual root lengths or the leaf area index (LAI). All these parameters can be measured only for models on a very large scale and thus only for very small areas. This shows that land use parameters – especially over long time periods – and also soil parameters cannot be gathered and recorded digitally for larger areas and long time periods. An application in the modeling systems is thus impossible at present and a spatially differentiated calculation of the infiltration rate or the groundwater recharge is also impossible. The advantages of those modeling systems are their applicability to high-resolution temporal data, e.g. daily values. Physical modeling tools are very appropriate for application in the unsaturated zone, below the soil and the influences of land use. Therefore, a segmentation of the modeling systems into a modeling system for the infiltration rate and a modelling system for the unsaturated zone is preferred for an integrated model.

3.2.3 Results of infiltration water modeling

The models for infiltration water result in spatially and temporally distributed data for the infiltration of soil into deeper layers. The soil is generally estimated to a thickness of about 2 m. The results can normally be saved and developed in a GIS without additional efforts, and from there on an exchange with other modeling systems, i.e., for unsaturated zone flow modeling, is possible. The techniques for coupling the data from static and dynamical modeling systems are applicable to various modeling systems.

An assessment of the results of modeling systems for the infiltration rate is difficult because experimental investigation and research can only be carried out in relatively small areas. The structural validity is fulfilled in all three types of modeling methods. However, the usual lysimeters cover an area of only a few m² and represent only a few selected types of land use and soils. Large lysimeters as in Eberswalde (Germany), and natural lysimeters can better serve for gathering comparable data. In most cases, the results are compared to the runoff measurements of surface water. This method is critical because there is a differentiation into different kinds of runoff that are measured at one point in an integrated way (surface runoff, interflow, base flow). In particular the spatial distributions of infiltration rates of very large model areas are extremely difficult to calibrate. The practical way of comparing the results of different modeling systems is systematically not allowed because the results are not obtained independently. Nevertheless, this approach is preferred to that of an uncalibrated model.

3.3 Modeling systems for the unsaturated zone



The modeling systems for the unsaturated zone under the soil zone are not considered in most cases because this zone is not very thick. For thin unsaturated zones, the infiltration rate is taken from the infiltration water models that are used directly as input for the groundwater recharge in a numerical groundwater modeling system for the saturated zone. Indeed, this procedure is reliable because in the unsaturated zone only retention and balancing of the groundwater recharge is observed in most cases. Only in rare modeling approaches must a horizontal flow in the unsaturated zone also be taken into consideration.

Of course, the modeling of the unsaturated zone can be connected by statistical methods to the modeling of infiltration water, either directly as part of the modeling approach or as an additional method. Some case studies, even for all of Germany, are documented by JANKIEWICZ ET AL. (2005), SZILAGYI ET AL. (2003), CHERKAUER & ANSARI (2005), and NEUMANN (2005). The methods that are generally calibrated by measurements of runoff are only suitable for predefined circumstances.

The application of a model for the unsaturated zone is necessary in some investigation areas and under special hydrogeological conditions, e.g. if layers with a low hydraulic conductivity cover the saturated zone and thus the infiltration of water to the groundwater is hindered. In this case, the horizontal flow, the interflow, must be calculated via an unsaturated zone modeling system that considers not only vertical flow but also horizontal flow. The interflow will increase the surface runoff. A perched aquifer with the same constellation will increase the groundwater recharge at another place, as described in GOSSEL ET AL. (2001). For these rare and complex hydrogeological situations, numerical 3D unsaturated zone modeling is necessary. Another case study by GOSSEL ET AL. (2009) describes the increased depth to groundwater in open pit lignite mining areas, where unsaturated zone modeling helps to calculate the time shift between infiltration and groundwater recharge.

Figure 18 shows the procedure of modeling the unsaturated zone. Even the input parameters show the complexity of this task. The precondition is a geological 3D model that must be parameterized for unsaturated zone modeling according to the model's purpose. For pure flow modeling the parameters are far less differentiated than they are in transport models.

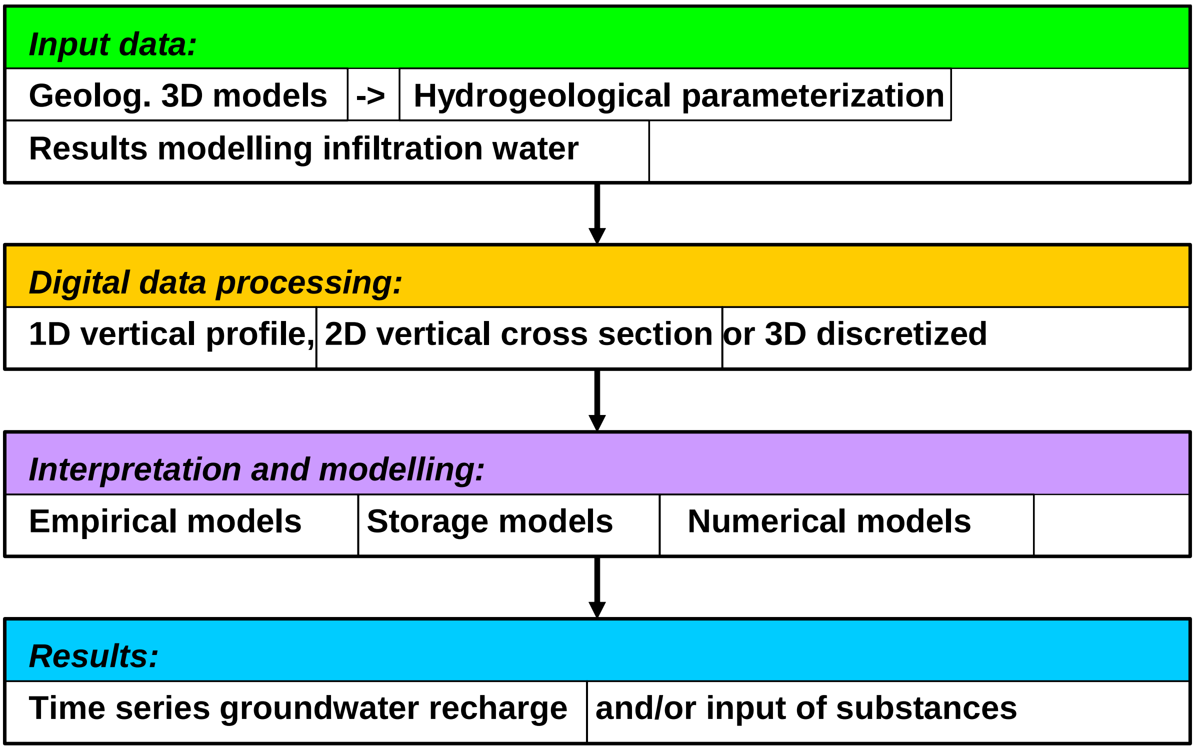


Figure 18: Modeling of the unsaturated zone. The vertical resolution of the geological models is not high enough to allow the numerical methods to obtain converging models. The increased vertical resolution in three dimensions leads to a multiplication of the elements of the horizontal resolution.

3.3.1 Input data for unsaturated zone modeling

If a detailed geological 3D model has already been developed, the structure of a numerical model for the unsaturated zone is already given. This way of connecting structures of models is also a way of coupling models. The model does not need any horizontal boundary conditions as long as the vertical flow dominates. Only in the case of interflow or perched aquifers, the horizontal extent of the model area should account for external conditions. The vertical extent is given by the definition of the unsaturated zone and can change dynamically in the case of high amplitude of the groundwater table. Problems for the parameterization of the unsaturated zone arise from the dependency of the vertical hydraulic conductivity (which is needed for flow and transport modeling) from the saturated hydraulic conductivity and the water content (MARSHALL ET AL. 1996).

Additional parameters for flow and transport modeling of the unsaturated zone are porosity, diffusion, dispersion, sorption, and biological degradation. Besides parameterization, the boundary conditions of the infiltration rate and the depth to groundwater should be considered, in addition to the initial conditions of the water saturation. According to BRONSTERT ET AL. (2005), this water saturation has a long memory effect that is especially apparent in global climate models (GCMs). BLÖSCHL (1996) demonstrates a similar effect for small catchment areas.

The equations and investigation results reported by VAN GENUCHTEN (1980) show that a parameterization can be carried out according to substrate descriptions. Even the initial conditions of water content can be estimated for a first attempt on this database. The influence of changes decreases rapidly with increasing calibration and with simulation time.

The vertical discretization of the unsaturated zone depends on the geological structure, on the thickness of the soil, and on the time-dependent fluctuating groundwater level. For most of the numerical modeling methods, the vertical resolution should be higher than the layer structure of the geological model on account of the convergence criteria.

3.3.2 Methods for the calculation of water flow in the unsaturated zone

Numerical modeling systems for the unsaturated zone are in most cases one dimensional, because flow and transport are restricted primarily to the vertical direction. The physical base of the numerical modeling systems for the unsaturated zone is the Richards equation, which is in most cases parameterized by the methods of van Genuchten and Mualem-van Genuchten (VAN GENUCHTEN 1980, VAN GENUCHTEN 1985, BOHNE ET AL. 1993, HOLZBECHER 1996, SYRING & KERSEBAUM 1988). Therefore, these modeling systems are classified as a combination of analytical and numerical methods.

If the unsaturated zone cannot be parameterized adequately, a statistical implementation may be the solution. In this case, the simplification of retention according to the thickness of the unsaturated zone is assumed for the infiltration of water. This behavior meets the flow processes only partially, but it can serve as a first attempt for many applications. Typical values for the infiltration velocity in glaciofluviatile sands were determined by GOSSEL (1999) to 1 m/d for the flow in areas with a small depth to groundwater. For the actual transport of water in the sense of a transport model, much longer time lags of about 1 month per meter must be calculated. Better data can be estimated via synthetic numerical models with 1D modeling systems (SIMUNEK ET AL. 2005). In applications of this modeling system, it can be shown that the results of the statistical analysis of GOSSEL (1999) can be applied only to the middle and fine sands of this investigation area. Saturation curves for other lithological conditions can be used for a one-dimensional estimation of the vertical flow velocity of infiltration water, and these values can serve as a better “statistical“ model.

A better simulation possibility is achieved by extending the storage models for the soil zone, the so-called bucket models, see chapter 3.2. In these modeling systems, a storage (“bucket“) is inserted for each layer. This “bucket” can be filled up to the field capacity. Additional infiltration water flows to the next “bucket”. The buckets are emptied either via evapotranspiration to the next higher bucket or via a slow flow into the next deeper bucket.

Transient numerical modeling of water flow in the unsaturated zone according to the Richards equation becomes unstable very quickly in a three-dimensional model. In areas with a thick unsaturated zone (>10 m), the water content decreases rapidly owing to the small amount of infiltration water as compared to the total porosity of the entire zone. No water percolates through this zone from a certain point on. The time step is defined by hydraulic conductivities, initial conditions, and infiltration rates. The hydraulic conductivities that are dependent on the water content, according to the Richards equation, are so small at this point that no more flow is possible. The observation of groundwater recharge, even in areas with large depths to groundwater, is connected to a preferential flow in these areas. These preferential flow paths lead to increased water saturation and, eventually, to higher conductivities in the surrounding area. In regards to feedback, this means that in the non-percolated areas, the flow of water is suppressed and the water must flow via the preferred paths. Inside of these preferential flow paths, the model can perform calculations using a hydraulic conductivity near the saturated value. Retention occurs as a result of the additional and slowly opening paths for water flow. These processes can only be modeled in very small investigation areas. For the regional scales in the proposed model areas, a very simplified modeling approach via a statistical model is therefore reasonable.

For the transport of substances in the unsaturated zone, the flow of water is assumed to be the most important process. On top of this approach the sorption process and the biological degradation are modeled. For the biological degradation, in most cases no dependencies and influences of different substances are considered, neither for the reactions between rocks and water nor for the questions of preferential flow or diffusion of volatile substances into the gas phase.

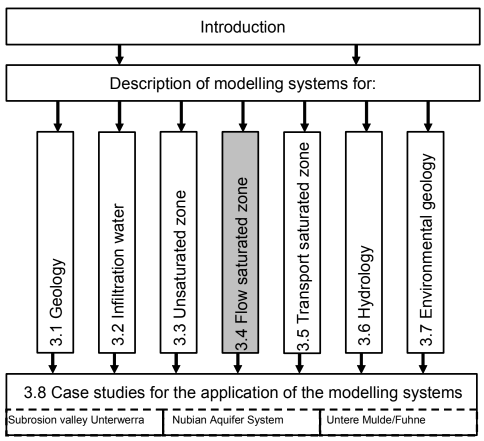
3.3.3 Results of flow and transport modeling in the unsaturated zone

In terms of using a bucket modeling system, the result seems to be quite easy to understand. The infiltration process needs time, and therefore a time shift is observed. Additionally, a smoothing of the output can be registered owing to the flow from one bucket to the next.

For modeling systems that are based on the physical Richards equation, the water contents for discrete elements are calculated. Thus, the volume of the water flow can be registered. This results not only in a time shift but also in a completely different curve for the discharge resulting from the changing parameters (e.g. for the hydraulic conductivity) during the simulation run.

An example of the role of processes in the unsaturated zone is given by RONEN & SOREK (2005).

3.4 Flow modeling systems for the saturated zone



In the context of the groundwater compartment, i.e. the saturated zone, flow-modeling systems were being developed in the 1960s and 1970s. The older analytical modeling systems, e.g. for analysis of aquifer tests, were developed mainly to obtain concrete physical parameters. Their application to modeling tasks is restricted to only a few special hydrogeological conditions. The first generally usable modeling tools were created through the use of electrical and electronic media. As a first step, analog models using resistivity paper were implemented, but these models had no chance of serving as a general modeling tool. In the late 1970s, computer systems became appropriate tools for a digital numerical implementation, and thus they allowed for a general application of the developed computer programs. Today, these numerical modeling tools dominate the calculation of groundwater flow and additionally, and they benefit from the development of visualization techniques.

As with modeling of infiltration water, the numerical groundwater modeling depends on hydrological input data, in addition to the geological and hydrogeological structures and parameters. They concern especially the inner and outer boundary conditions and the groundwater recharge. The whole preparation procedure is described by the term “Conceptual Hydrogeological Model”. These interdependencies of several modeling systems demonstrate the necessity of diverse couplings of modeling systems. The interfaces for this process are described in chapter 4.

The modeling tools are in most cases divided into a preprocessor and a postprocessor in order to visualize the input and output data. The main calculation is performed by a highly optimized kernel.

The modeling process as shown in Figure 19 is a complex procedure. It depends on the abstraction of the geological model toward a hydrogeological structural model with a preliminary parameterization. The results are usable for diverse modeling tasks. For the entire modeling process, a GIS can be used as a server for data input. The preprocessors and postprocessors in most recent modeling tools have direct interfaces for GIS data import and export.

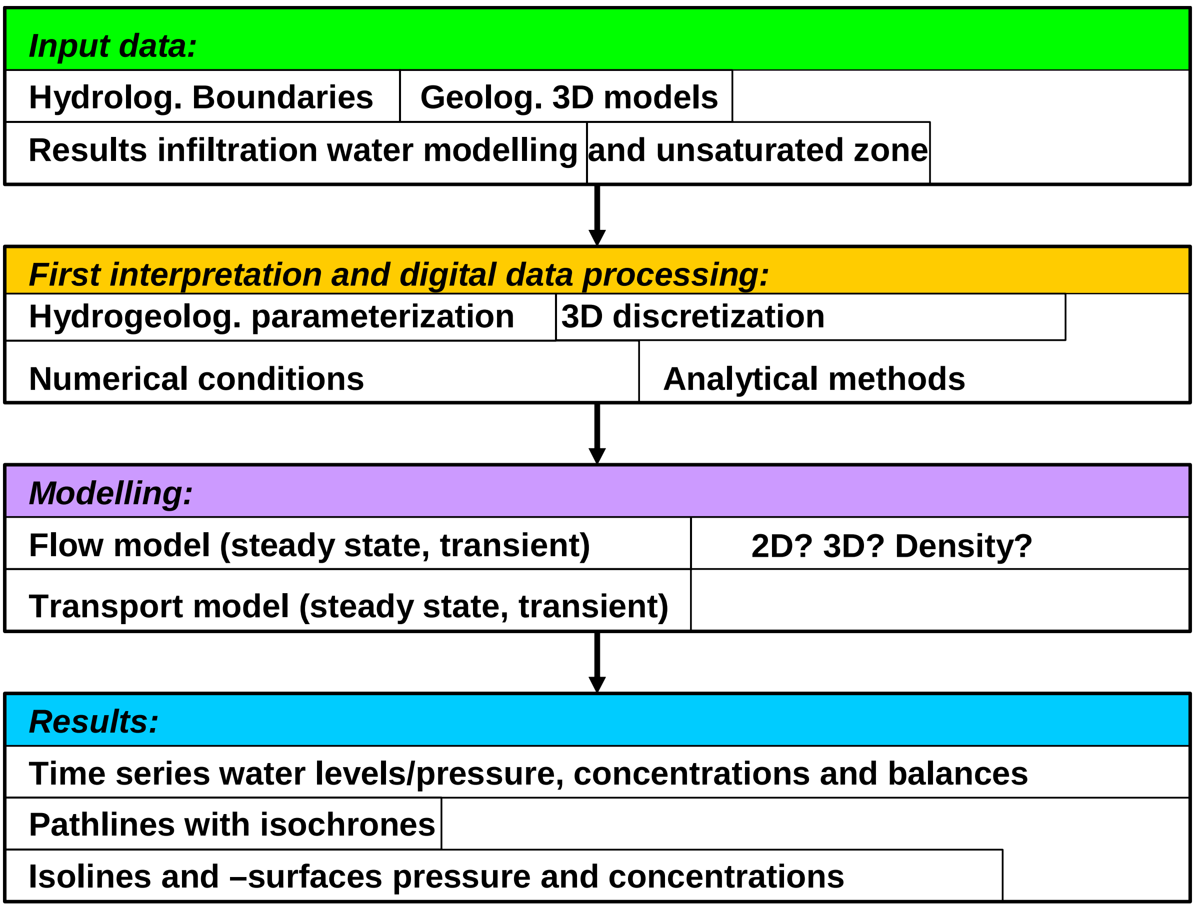


Figure 19: Modeling of the saturated zone. The modeling methods can only be used if the input data for the model are prepared in advance by additional processes.

3.4.1 Input data of flow modeling systems for the saturated zone

The input data of the numerical groundwater modeling depends on the dynamical status of the model. Steady state models and transient models differ at least in terms of boundary conditions and parameters. Sometimes even the solvers differ in steady state and transient models.

The simplest case of a steady state flow model uses structures and parameters as input data. Ideally, this data can be derived from the geological model (see chapter 3). The most significant differences to the geological modeling process are the horizontal dimensioning of the numerical flow model and the adherence to the boundary conditions, which must be derived from a hydrological concept in most cases. In some cases, the outline can also be bound to geological structures. In the third dimension, geology is dominating the discretization of the model via the structure of layers converted to aquifers and non-aquifers. The temporal dimension is bound to the dynamical conditions of hydrological and technical values. The static character of the geological model does not play a role in the time dependency of the model. Hydrological values to be considered are hydrographs of surface water (boundary conditions) and groundwater recharge (parameters and boundary conditions), whereas the technical values are groundwater extraction, etc.

The structures of a numerical groundwater model can be generated in very different ways. HUBERT (2011) gives a detailed explanation and analysis of the implemented methods.

The hydrogeological parameters are derived in most cases from the lithological description. Another option is the interpolation of measured data, e.g. from aquifer tests or from slug & bail tests. Regarding derivation from lithological descriptions, e.g. borehole logging, preliminary interpolation via indices is most advantageous. For the calibration of the model (see chapter 4), these indices can be varied slightly and in a reasonable range, and interpolation of the parameters is started again based on the new dataset. The behavior of different hydrogeological parameters must be obeyed in the interpolation process. Hydraulic conductivities should be interpolated in most cases in a logarithmic form after the relation has been proven by a statistical analysis of the values. Porosities are interpolated linearly in most cases. Here, the dependency of the burial depth can be accounted for by an empirical formula. The groundwater recharge can be interpolated only in the temporal dimension because a spatial interpolation (e.g. of lysimeter data) does not make sense considering that the dependencies from land use, soil, and depth to groundwater dominate the recharge process, as described in chapter 3.2. For data exchange, the problem arises that the recharge hydrograph sets the values for daily recharge in a whole month or, in the case of boundary conditions, the surface water levels as a mean value for a whole month. This must be considered in the coupling process. The setting of the groundwater recharge as a parameter is discussed because its possible time dependency in transient groundwater models is interpreted in several modeling tools as a hidden boundary condition. Thus, it can sometimes be found there as well.

The boundary conditions are set time dependent in most transient models. They should be treated in different ways: Predefined water levels, e.g. hydrographs of surface water, must be interpolated linearly and in the temporal dimension. In these cases (and in contrast to the interpolation of groundwater recharge), simple linear interpolation methods can be adopted. Watersheds can be used as boundary conditions (no flow boundary) if they are stable and constant in time. Geological structures are usable (though only rarely) in real model areas, e.g. in the case of basement outcrops as described in GOSSEL ET AL. (2004). As shown in chapter 3.8.1 and LÄHNE (in preparation), boundaries of hard rocks cannot be used as boundary conditions in every case.

Parameters, as well as boundary conditions and initial conditions of the numerical groundwater models, can be recorded and handled by GIS. GOSSEL ET AL. (2004) show that for this task, pure GIS functions, e.g. the spatial database management for large datasets, are not only functions that can be applied. Additional and subordinately developed and integrated GIS functions, such as interpolation control functions of spatial datasets and capabilities for data exchange, are used in this process intensively. It is problematic to handle real 3D data that should be determined by geological modeling tools and time dependent data such as the groundwater recharge. For both, a highly differentiated data management is possible in GISs. However, these additional data structures are necessary for the modeling process, and data exchange is not originally implemented in GISs.

3.4.2 Methods of modeling systems

The physical fundamentals of the numerical groundwater flow modeling are the continuity equation and the Darcy equation. Combining these equations results in a partial differential equation that allows for the calculation of groundwater levels in porous media.

For the solution of the partial differential equation, finite difference (FD) and finite element (FE) methods are typically applied. Finite volume methods are not nearly as widespread as FE and FD methods. In these modeling systems, space and time are discretized so that, for each element, a consistent dataset of spatially and temporally constant values is created. Via the discretization, the partial differential equations are linearized and thus these numerical methods are only approximations – but with a predefined approximation value. The discretization can be accomplished with readily available computer capacities and modeling tools, so that procedures and models become quasi-continuous. Detailed examples for the generation of modeling tools from the described modeling systems can be found in DIERSCH (1984), KINZELBACH (1986), and MCDONALD & HARBAUGH (1988). In the horizontal direction, the model area is discretized into rectangles, irregular quadrangles, or (irregular) triangles. In the vertical direction, all modeling tools work with layers or slices that must be maintained in the entire model area. The only possibility of creating geological lenses or fading out layers comes from working with inserts that divide a couple of cells automatically, either in the vertical or in the horizontal direction (this is in contrast to a pure mesh refinement). The elements in the horizontal direction are thus extended in the vertical direction to prisms or (irregular) cubes. This structure simplifies exchange of the slices using either TINs (triangular irregular networks) or GRIDs, but it is complicated when adopting all geological structures and units.

The geometries of the elements definitely influence the behavior of a model. In triangular nets (or meshes), as few triangles as possible should have angles > 90° because models with many such triangles will converge only after numerous iteration steps. The problem becomes even worse in transport modeling. For all numerical modeling systems, it is important to realize that there are upper limits to the extent of elements and time steps (Courant number and Péclet number). This prevents divergence of the model. In flow modeling, this danger is relatively small in contrast to the situation in transport modeling of groundwater. The same problem arises if the thickness of the layers is too small. This will lead to numerical divergence.

The internal algorithms must be investigated – and therefore documented – very thoroughly. As an example, averaging of hydraulic conductivities between neighboring cells or elements leads to completely different results depending on which mean – arithmetic or harmonic – is used. With an arithmetic mean, the cells with low hydraulic conductivity become much more conductive after the averaging. When using a harmonic mean, the cells with high conductivity become much less conductive after averaging. This is of little significance for the flow in the horizontal direction because the discretization can be increased slightly to avoid this effect. In the vertical direction, a higher resolution dramatically increases the number of cells/elements because it is multiplied by the number of cells in the horizontal direction.

The reduction of most groundwater flow modeling tools to the saturated zone is problematic in the case of transient models of unconfined aquifers. If the uppermost cells become dry, rewetting sometimes is not possible owing to numerical reasons. This leads to (very small) differences in the results of modeling tools that have strategies for avoiding these problems.

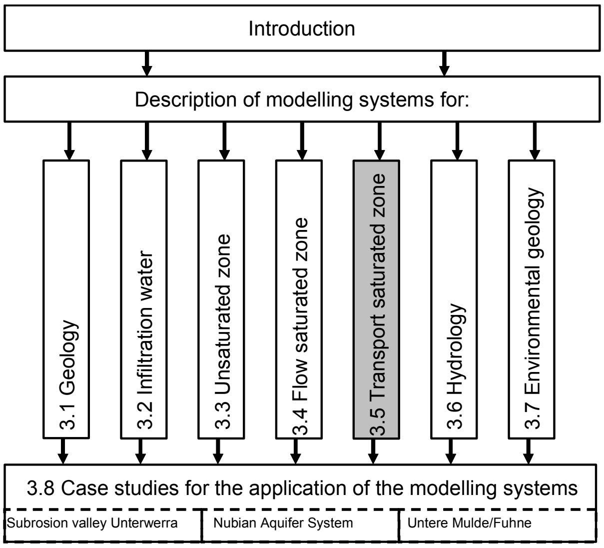
3.4.3 Results of numerical groundwater flow modeling

Numerical groundwater flow models are used for a wide variety of modeling tasks. Consequently, the results are quite diverse. Pure groundwater flow models (steady state or transient) are used for water budget modeling and for predicting the effects of human activities on water balances, flow regimes, etc. Balancing for the whole model area, or for selected parts of it, is readily accomplished through the calculation of water balances for each element/cell/node, and thus this task is implemented in all modeling tools. The same principle is used for the calculation of water levels. The water levels are connected by the basic equations to the balances, and therefore these values can be obtained from the model, using a 3D model for each of the model layers.

Based on the gradients between the single cells/elements, path lines can also be calculated. Because of the physical basis and the definition of path lines, only the path of so-called representative elementary volumes (REV) can be calculated. For such REVs, all parameters of the cells/elements are constant and forma continuum. The calculation of the paths through the pores cannot be calculated with the continuum approach, but this normally is no serious disadvantage. In three-dimensional groundwater flow, models of the path lines can be calculated for one model state in three dimensions, and they can be calculated as transient path lines in a connection of the flow states after the complete transient flow modeling if all time steps have been recorded.

GISs seem to be well suited to visualization of the results because they have the capabilities for handling the necessary interpolation methods. The original features of GISs, such as spatial reference systems and 2D visualization possibilities, make them most convenient for presenting the results in the form of maps. For 3D visualizations (e.g. for path lines and distributions of pressure), and for 4D data, (e.g. decreasing or increasing groundwater tables over time) GISs are usually not suitable. Only a few scientific GIS tools are capable of and specialized in such data handling.

3.5 Transport modeling systems for the saturated zone



For the saturated zone, transport modeling systems are available in addition to the flow modeling systems to which they are coupled. These systems are needed for advective transport modeling with the water in the REV, and they also include models for the processes of diffusion, dispersion, sorption, and degradation (biodegradation or radioactive decay, realized by a decay rate). These processes lead to a complex database that is not only bound to spatial distributions but also scale dependent.

The objectives of transport modeling in the saturated zone are very diverse and include the assessment of groundwater contamination and remediation possibilities, retention, time calculations in the catchment areas of drinking water supplies and predictive modeling in the case of environmental impact assessment.

Steady state or transient transport models can be coupled to transient or steady state flow models. Coupling a transient flow model to a steady state transport model, however, does not make sense.

The input parameters of numerical transport models can be, as mentioned above, very complex and diverse. The diffusion must be regarded only as a temperature-driven process and as specific to a certain substance if the combination with other substances in groundwater models is to be neglected in the diffusion process on account of the low concentration of contaminants. In contrast, the parameters of dispersion, sorption and decay are very complex and, in most cases, are not experimentally measurable. Therefore, groundwater transport modeling in particular exhibits a significant contrast between the database and the diversity of tasks for which it should be used.

The dispersion process can be divided into a grain-sized dispersion and into macro dispersion. KINZELBACH (1987) distinguishes these two processes because macro dispersion is mainly scale dependent, i.e., on a local scale and with a high spatial resolution the macro dispersion is low, and in regional models with a lower spatial resolution, the macro dispersion increases. Considering this behavior, the possibilities for an experimental measurement of the macro dispersion are very restricted. Whereas the grain-sized dispersion can be measured even in the field via aquifer tests or long-term groundwater monitoring, the macro dispersion can only be estimated according to the variability of hydraulic conductivities in the model layers, this is the most important influence for this value.

The sorption of substances has the role of retardation in the whole transport process. This can be regarded, to a certain extent, as constant in each model layer. Exceptions are layers with varying contents of clay and organic detritus. This parameter can also be measured in the laboratory quite well, and additionally a measurement via aquifer tests is possible.

In most numerical modeling systems, the decay of substances is treated like radioactive decay via a half-life parameter. Some problems arise for this method if the decay is dependent on the availability of other dissolved substances, e.g. oxidizers as there are O_2, NO_3^-, and SO_4^{2-}. This dependency cannot be covered by a simple decay rate or a half-life value, rather, it must be modeled via special modeling systems for reactive transport according to the mass balance equation or in a kinetic modeling approach. Some modeling tools explicitly serve the interfaces for a coupling of both systems (see chapter 3).

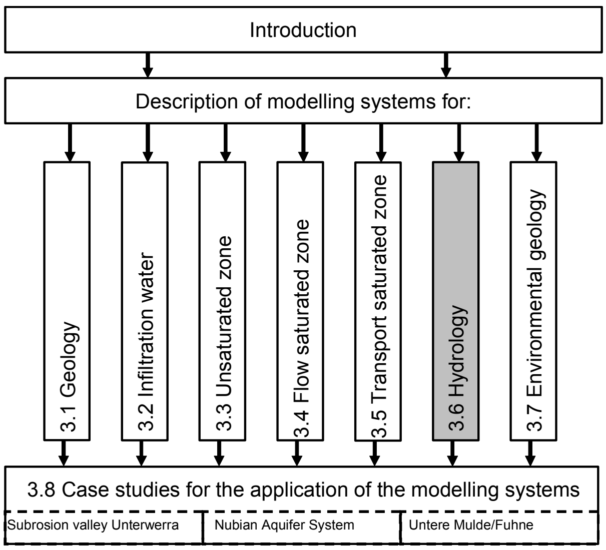
The theoretical basis and methods for transport modeling are described in detail by DIERSCH (1984) and KINZELBACH (1987). In practice, the transport modeling is sensitive to complex geometries and low resolutions. For the spatial discretization, the Péclet-number must be obeyed in order to avoid an apparent numerical dispersion. This apparent numerical dispersion is based on steep concentration gradients that can be avoided by using a higher spatial or temporal discretization. For the temporal dimension, the Courant number has the same function.

The results of the transport modeling can be visualized in a 2D environment via a GIS very comfortably. For 3D and 4D visualizations, e.g. iso-surfaces of concentrations with a temporal dimension in the case of transient modeling, GISs are not suitable. In these cases, the postprocessor for the modeling tools must be used to create animated film sequences.

For transport modeling in groundwater, a question arises, as to whether multispecies transport should be considered. Most of the modeling systems have the capability of modeling at least a few predefined or self-defined reactions via a kinetic approach. The reaction terms and equations of equilibrium modeling approaches are so complex that there are several separate tools for hydrochemical reaction modeling. The most prominent tool is PhreeqC (PARKHURST & APPELO 1999). In the case studies, transport modeling with separate tools was not carried out; and thus the modeling tools are not further described here.

3.6 Hydrological modeling systems: Atmospheric input and modeling systems for surface water

Regarding hydrological modeling systems, several compartments that have a larger range than do those of geological and hydrogeological modeling systems should be identified. The palette of hydrological modeling systems is more extensive owing to the wider array of modeling tasks and the larger number of considered compartments.



Classical hydrological modeling systems, especially catchment models, are of minor interest for hydrogeological modeling. In most cases, these modeling systems use statistical methods for such things as rainfall-runoff modeling of a catchment area, hydrological subsystems such as snow melt or the dependencies between topography and rainfall. In other cases, the runoff in a riverbed is modeled with numerical methods. The statistical method of the separation of significant patterns in hydrographs, and thus also the calculation of the base flow, helps to calibrate groundwater recharge models.

Other models work with couplings of modeling systems of different kinds. They are of special interest because of their systematic structure and behavior. In these modeling tools, which are constructed from several subsystems, deterministic and statistic concepts are mixed in different proportions to make a tool that is easy to handle and that offers a high functionality.

The scale is most important for the work with hydrological modeling systems. For example, the dependency of rainfall on topographical height and exposure to the main wind direction was worked into a statistically significant model by HUTCHINSON (1995) and HUTCHINSON (1998). These phenomena observed in large and/or mid-range areas are not reproducible in global climate models or water balance models (DÖLL ET AL. 1998). Using examples, BERNARD (2005) shows how models of small areas (maximum regional scale models) can be supported by a GIS in the preprocessing and postprocessing. Problems arise from the deficiencies in 3D and 4D support in the GIS systems. These problems have already been discussed in reference to numerical groundwater modeling. The capabilities of different GISs vary widely, and some specialized are designed to close these gaps. OpenSource GISs are more developed than commercial standard GISs, and they allow users to add their own features.

FÜRST (2004) uses GISs for applications in water management and hydrological modeling. The details and the pros and cons of vector-based GISs and raster-based GISs are discussed in a hydrological context. In practice, a mixture of both concepts (a so-called hybrid GIS) and the frequent change of data formats dominate the modeling procedure as is pointed out in the case studies. According to FÜRST (2004), spatial variability of hydrological models can be better obtained by the application of a GIS than by using the most original modeling tools. Modeling systems of a very low dimensionality, e.g. zero-dimensional catchment modeling systems and one-dimensional modeling systems for pipes and rivers, play an important role in hydrological modeling. For these systems, the application of a GIS offers no advantages. FÜRST (2004) classifies the modeling systems for runoff analysis and simulation as follows:

- Spatially aggregated modeling systems for flooding prediction (e.g. based on the method of unit hydrographs).
- Spatially half-distributed modeling systems for regional scale catchment areas.
- Spatially distributed modeling systems, process-oriented runoff modeling systems.

These modeling systems are supported by GIS methods in different ways.

Spatially aggregated modeling systems can be supplied by the digital elevation model of the area and by land use-specific parameters, e.g. asperity. For this purpose, in some GIS extensions, additional routines are predefined. In spatially aggregated modeling systems, statistical methods not only are applied for the spatial aggregation procedure but also are an important part of the modeling concept itself.

Differentiating between spatially distributed, aggregated, and spatially half-distributed modeling systems is difficult in most cases because the transitions between them are continuous. Additionally modeling systems for different compartments can obtain input data from a GIS in diverse forms. Most characteristic of these modeling systems is the segmentation of the space into different compartments (e.g. snow coverage, interception at the surface of plants, diverse soil compartments) that are in most cases implemented by storage functions. Areas and volumes of these storage values can be used for calculations via the discretization capabilities of a GIS. In this process, concepts known as hydrological response units (HRUs) are used to summarize areas with the same hydrological parameterization and behavior in order to dramatically reduce the processing effort (see chapter 3.2). Spatially half-distributed modeling systems are thus implementations of the classical stochastic modeling systems with varying portions of statistical and deterministic modeling concepts.

Spatially distributed modeling systems extend the systematic analysis and application of hydrological concepts in the direction of deterministic and physically based modeling concepts. They consider the pure water balances and the erosion and sedimentation processes induced by runoff. Because of the complexity of this process, modeling and the high-resolution data needed for the input to the application are restricted in most case studies to very small selected areas.

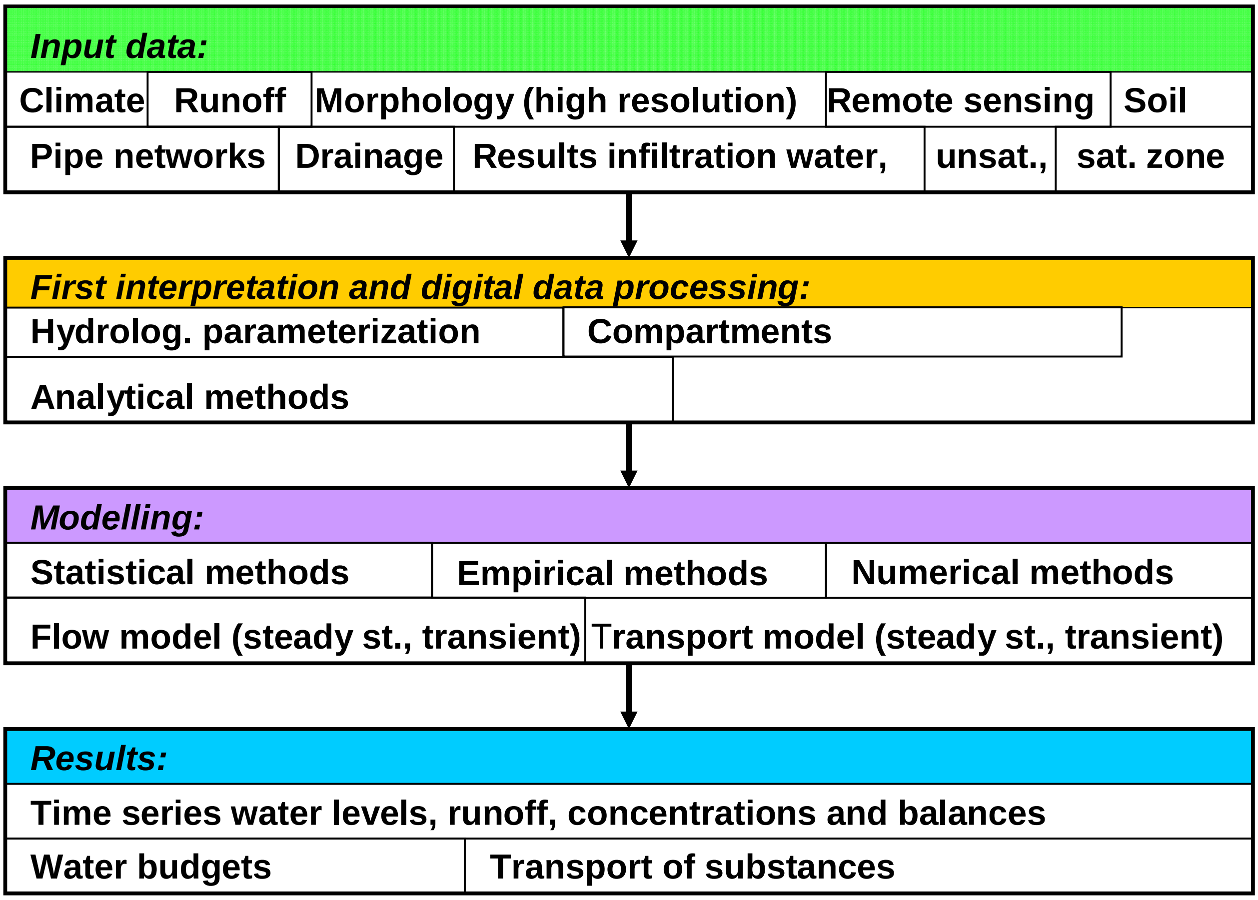


Figure 20: Hydrological modeling. The spectrum of the modeling systems is very diverse and only a selection of it can be presented here. The spectrum is similar for input data and results.

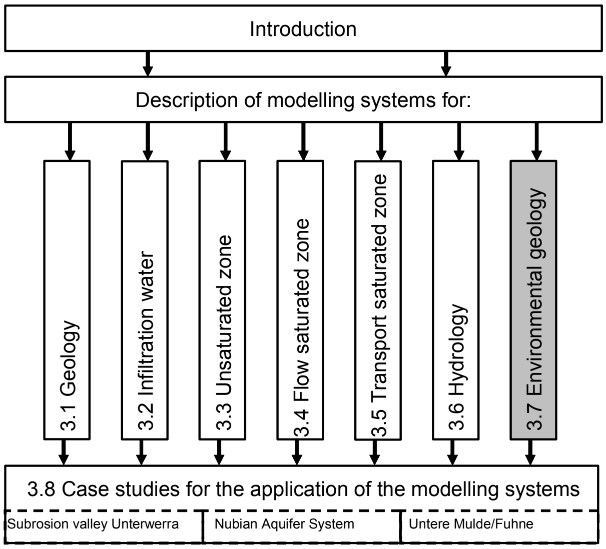
For climatic investigations over long periods, four kinds of modeling systems are applied (VALDES 2005):

- Box models that work mainly on a statistical basis.
- Energy budget models that are based on the modeling of energetic processes.

- Climatic models of medium complexity (Earth System Models of Intermediate Complexity, EMICs), which calculate energy balances and single processes such as circulations in oceans and the atmosphere.
- General Circulation Models (GCMs), which implement the dynamical basic equations completely.

While the calculations in the first three modeling systems can be performed quickly, GCMs require very high computing capacities owing to the large number of input parameters, the diversity of the modeled processes, and the spatial and temporal resolution.

3.7 Modeling systems in environmental geology



Modeling in environmental geology creates the possibility of a summarized and proceeding analysis. The modeling systems for these purposes are in most cases not standardized, and the tools are not ready for use. Exceptions are the assessment tools for a risk-based assessment of certain contaminations and the systems used for the assessment of aquifer vulnerability or groundwater protection. In fact, special algorithms must be developed based on general tools, such as a GIS.

The following examples for modeling in environmental geology only provide an extract of the most discussed and most commonly used applications in this field.

Erosion and sedimentation processes of soils can be modeled by the well-developed methods of the universal soil loss equation (USLE). This conceptual modeling method can be implemented in modeling systems and tools. FÜRST (2004) presents the results of such models in alpidic areas that were built on distributed parameters and GIS methods.

For a decision support system (DSS) the opportunities that are introduced by GIS are important in several ways:

- Data supply
- Visualization (preprocessing and postprocessing)
- Data exchange with and between specialized modeling systems
- Implementation of DSS-specific functions
- Implementation of well-known user interfaces

In addition, in this case, the restrictions of GIS in terms of handling spatial and temporal data must be taken into consideration. With few exceptions, GISs are not capable of handling and serving volumetric 3D datasets or of adequately modeling transient data.

The interpolation methods that are available in most GISs are important tools for modeling in environmental geology. For a discussion of the tools and methods that are widely used in geosciences, the detailed explanations referenced in chapter 2.1.1 should be sufficient. In addition to geological structures hydrochemical analyses can be interpolated by these tools. Problems arise only in the combination of both results with a geologically adjusted distribution of substances. For distributions according to hydrological processes, the same problems should be mentioned. The application of static models leads to another difficulty, namely, the necessity of considering samples of different sampling times; this is generally solved through insufficient averaging. For a systematically acceptable solution of this problem, only the connection to dynamical modeling systems is reasonable, although a reduction to a certain time chart may also be suitable.

The modeling systems that can be connected for models of environmental geology are found in all kinds of dynamical modeling systems, but the preferred modeling techniques were developed in ecology and economy:

- Groundwater modeling
- Surface water modeling, especially runoff and quality models
- Groundwater recharge modeling
- 3D geological modeling

For the modeling tasks in environmental geology, a number of additional applications for connected modeling systems should be considered (see Figure 21). In the fields of nature conservancy and protection, agriculture, economics, and tourism, mostly new adjusted and developed conceptual models can be implemented with GIS methods because standard modeling systems are often lacking in these fields. Modeling systems of the social sciences are rarely applied to or implemented in DSS. The results of these models must be communicated in a much wider range as compared to most of the other modeling results. The involved parties (NGOs, agriculture, economics, and tourism) also want to know about the uses of the data they submitted. Special methods, including map server applications, need to be developed to meet this intense interest. STEINMETZ (2007) showed that handling a mixture of protected and free data is quite complex. Another difficult question is whether basic data itself, derived data or no data at all for a certain topic should be accessible.

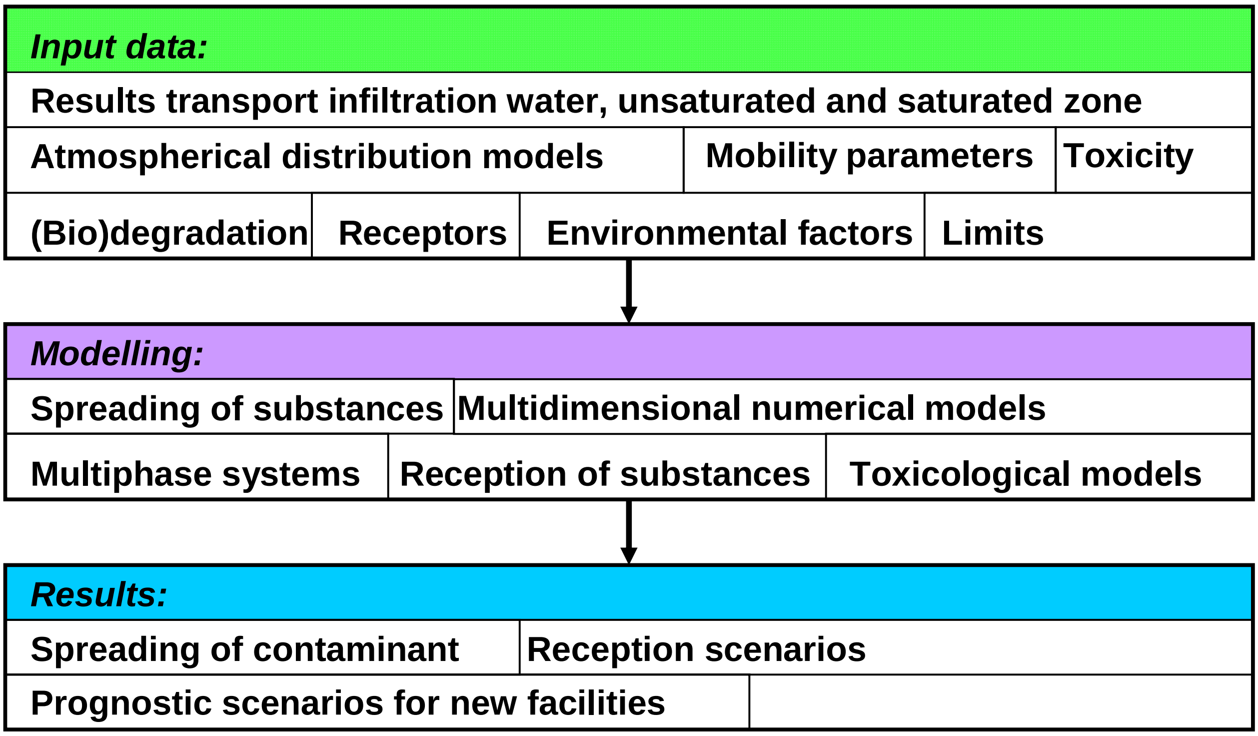
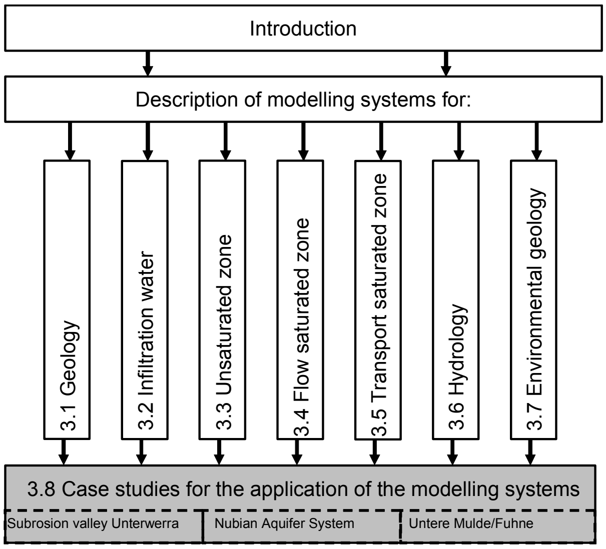


Figure 21: Modeling in environmental geology. While ready-to-use (or ready-to-implement) modeling systems are available only for special objectives, the modeling tasks, results, and kinds of data can vary widely.

3.8 The applications of modeling systems in the case studies



In addition to the case studies that are described in detail, some examples from the literature are also presented to demonstrate the diversity of the applications of modeling systems.

The areas of influence for groundwater observation wells can be outlined only by transient three-dimensional modeling of the saturated zone. After the first investigations in this field, which were carried out in the context of a research project (ZEUS) at a research institute in Ulm from 1993 to 1995, it became necessary to choose a solution with a 2D numerical approximation and an analytical solution. This approximation could only be used under certain conditions and after 3D numerical tools and better computers had been developed; this first approach was rejected. For several thousand groundwater observation wells, strategies for a numerical 3D modeling were developed. For the modeling tasks described in GOSSEL ET AL. (1998) and GOSSEL ET AL. (2001) these questions were handled for regional groundwater catchment areas. To calculate retention times of substances in groundwater, it is necessary not only to calculate path lines but also to model the transport processes, even if it is only for an ideal tracer that accounts for the porosities or storage coefficients and dispersion. This is important not only for the spreading and distribution of groundwater contaminants from hazardous waste dumps and cases of water pollution but also for the observation of groundwater quality, especially in the catchment areas of the drinking water supply. BENDER (2003) shows an example of this for a regional model in the area between the Rhine and the Neckar. The modeling tasks are extremely complex for cases of assessing natural attenuation processes in polluted areas or remediation areas, as PRECHTEL ET AL. (2003) point out. Other important fields for the application of numerical groundwater models are environmental impact assessments and groundwater management for large buildings.

For most of these models of the saturated zone, no dedicated geological models are developed. In these cases, the hydrogeological structural model is directly built on the basis of a few field data and the rough hydrogeological structure of aquifers and aquifuges. Models for infiltration water and groundwater recharge, as given in WEGEHENKEL & SELG (2002), are applied to the water balance calculations in the context of permissions for groundwater extraction for drinking water, industrial water, or service water (JOSOPAIT 1996). In the context of general environmental reports and/or public participation, these results are also published by either the stakeholders or the authorities.

3.8.1 Subrosion valley Unterwerra

The geological model of this area was created using constructive methods, as described by LÄHNE ET AL. (2006). In Figure 22 the overall workflow of the modeling process is shown. The necessity of a detailed DEM in this procedure is clear. The stratigraphical classification of geological layers is very simple in this area because the lithology of the hardrocks from the Upper Permian (Zechstein, halites, and gypsum), the Lower Trias (Buntsandstein/Bunter: sandstone, siltstone, and claystone), and the Middle Trias (Muschelkalk: limestone) are easy to recognize in the field. Furthermore this area was investigated in detail by the geological mapping project JACOBSHAGEN (1993) and by a study that employed special facial analyses (WYCISK 1984). The geological structures seem to be very simple because the layers are only bent as flexure zones. Also, some rare faults vertically disturb these simple structures, but these effects are less important. The Quaternary layers in the valley that reach a larger thickness (> 2 m) are also easy to stratify and are horizontally persistent.

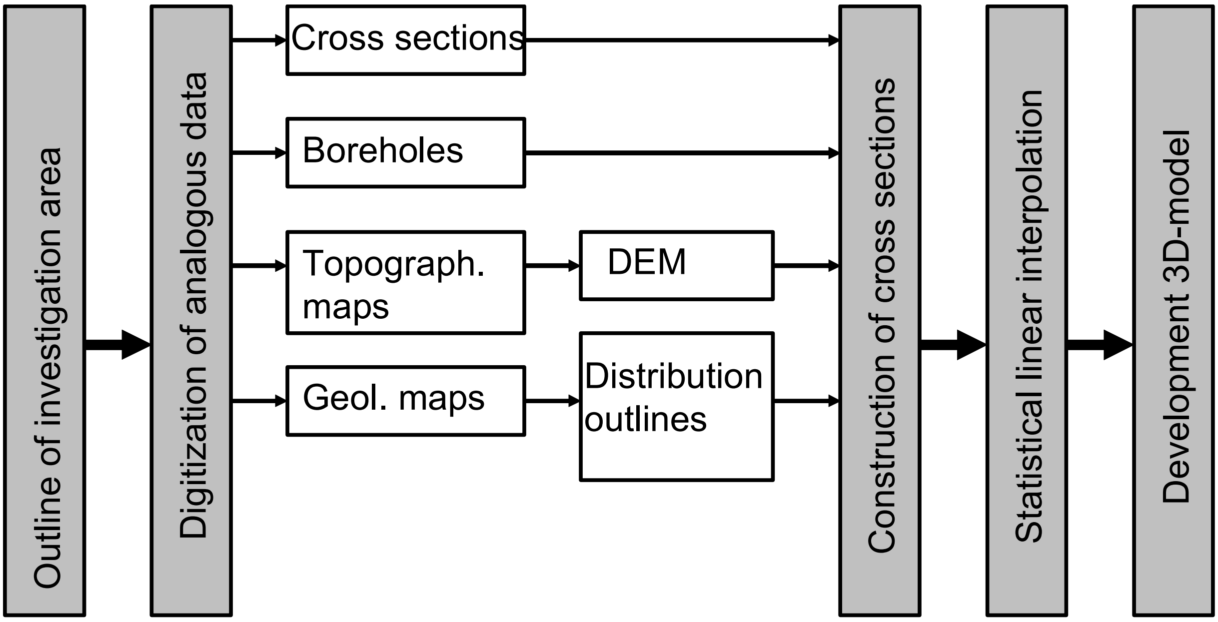


Figure 22: Workflow of the geological model for the subrosion valley Unterwerra.

Analytical methods have been applied intensively in this area owing to a high density of groundwater observation wells; this, along with the numerous field courses, led to a very accurate calculation of hydrogeological parameters. This was very advantageous for the hydrogeological assessment of the processes in this area. These methods, and the results of their application, can serve only to a minor extent for the solution of complex objectives because they can be applied only under excessively simplified conditions. Together with the geometrical analyses of dynamical measurements, e.g. of groundwater levels and hydrochemical data, they were used to generate an initial dynamical image (LÄHNE 2003). This overview was used in the following process as part of the conceptual dynamical model. Figure 23 shows the exceedingly high density of hydrogeological and hydrological observation points used for the calculation of hydrogeological parameters in the valley. These values can be used as input data for a numerical groundwater flow model in a rather statistical way, without the need of further geological investigations or additional geological knowledge.

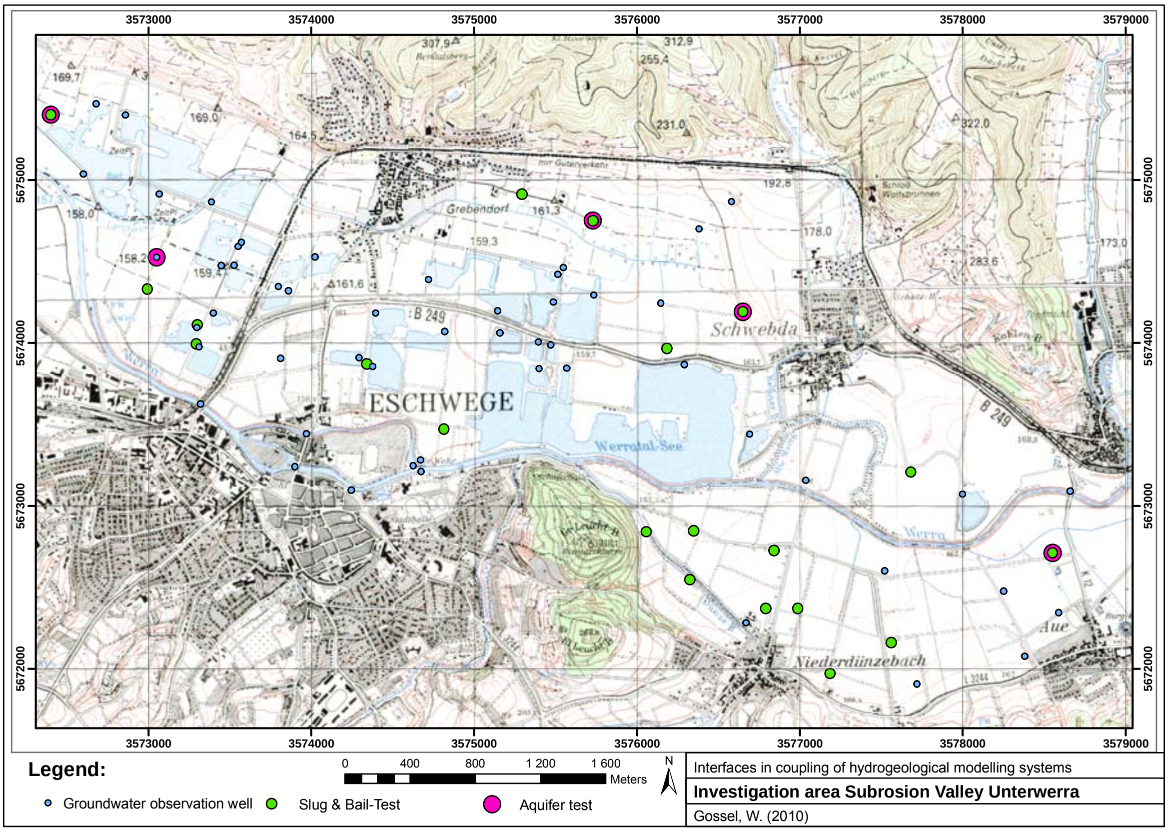


Figure 23: Map of the hydrogeological investigations in the subrosion valley Unterwerra for the analytical determination of hydraulic parameters. The observation wells are used also for hydrochemical analyses.

Another striking feature of this investigation area (beneath the high density of observation points in the valley) is the inclusion of hard rock areas (especially Upper Permian and Lower and Middle Trias) in the numerical hydrogeological modeling approach. This is done because these areas belong to the catchment area of this part of the river Werra, and the recharge processes from the hard rock areas to the valley are not easy to identify. The continuum approach was employed because there were no dominant or preferential flows observed from the hard rock areas to the Quaternary aquifer in the valley. The workflow in Figure 24 depicts the use of the analyzed data in detail.

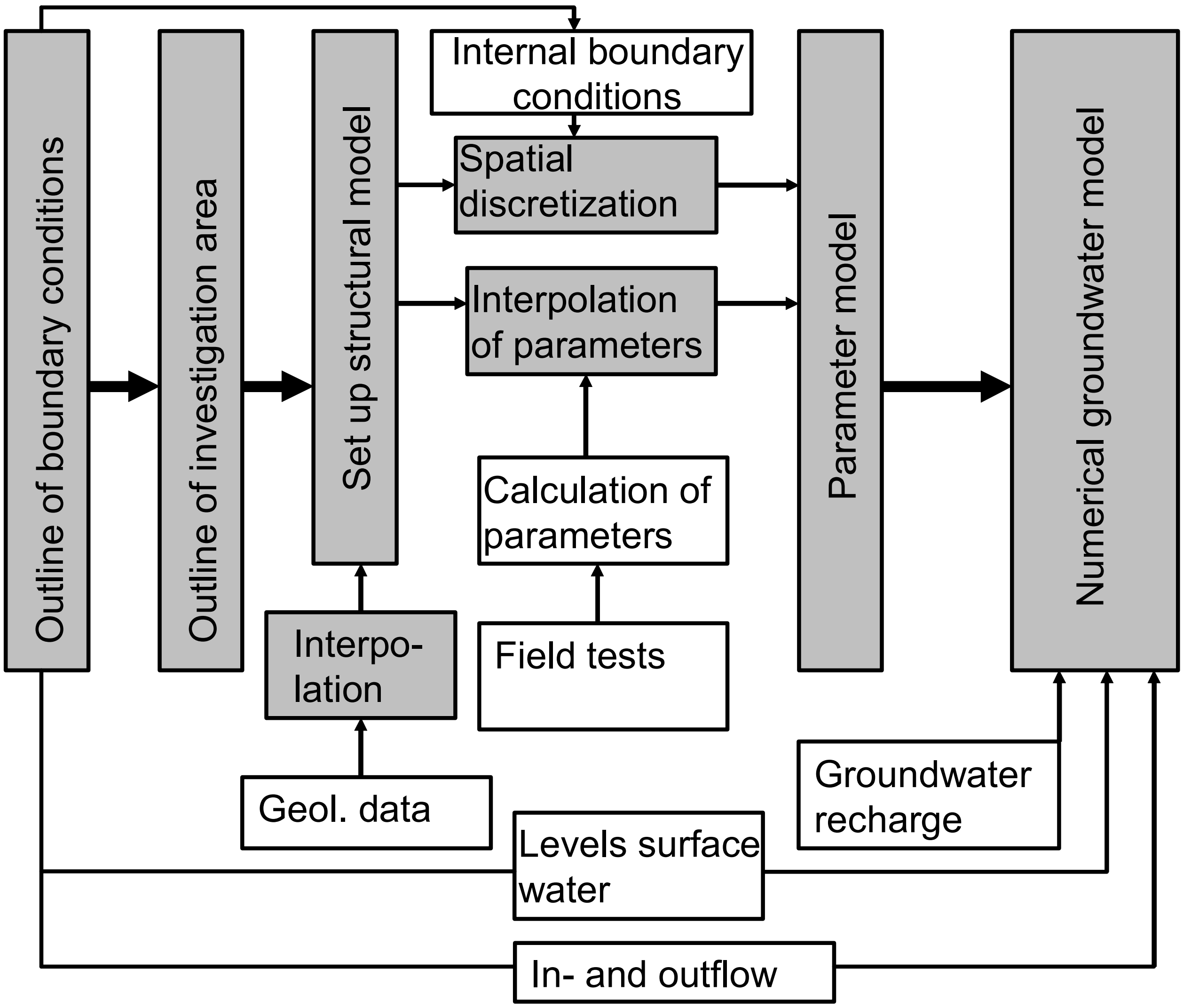


Figure 24: Workflow of the numerical groundwater modeling for the subrosion valley Unter-werra.

Coupling the geological model to the numerical groundwater model is a significant challenge because the soft rocks in the Quaternary aquifers in the valley do not exist in most parts of the catchment. They are the most important hydrogeological unit in this area, and they, rather than the hard rocks, dominate the flow regime.

The groundwater recharge was calculated according to the method of TUB-BGR (WESSOLEK ET AL. 2004). Developing the model of a hypothetical groundwater surface in the hard rock areas, which was needed for the calculation of the depth to groundwater, was most challenging. As shown in Figure 25 this task plays a central role in groundwater recharge modeling.

A modeling system for the unsaturated zone was not applied in this area.

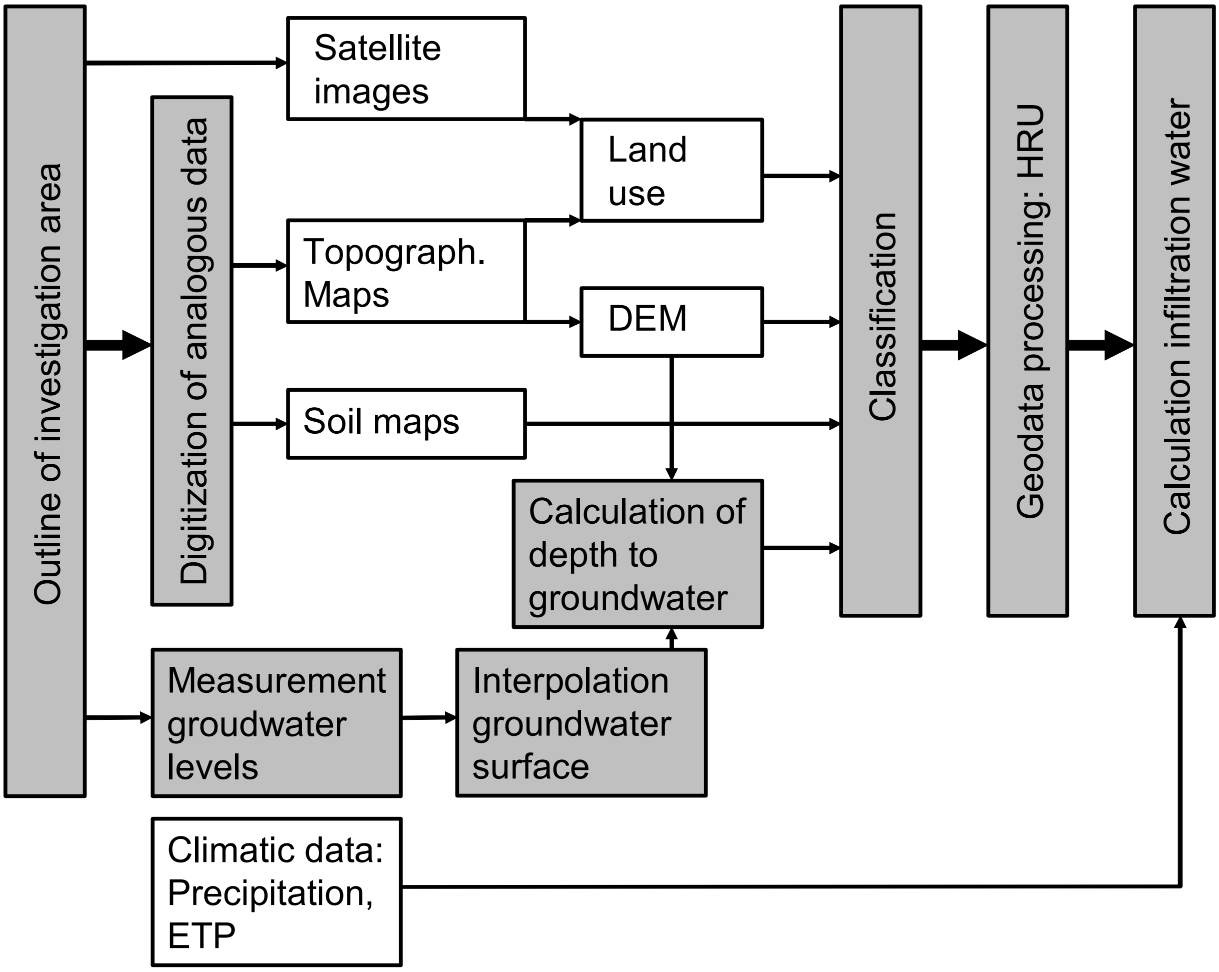


Figure 25: Workflow of the groundwater recharge modeling for the subrosion valley Unterwerra.

3.8.2 Nubian Aquifer System

The geological modeling for the Nubian Aquifer System was carried out in a simplified way because the focus of the modeling was the numerical groundwater model (see chapter 2.4.2 and Figure 26. The input data were gathered from a wide variety of publicly available data, e.g. borehole information and geological cross sections reported in BRINKMANN & HEINL (1986), the geological map (CONOCO 1987), the map of the top of the basement (HESSE ET AL. 1987), and the DEM (NASA 2005). All these data were georeferentiated and digitized to establish a consistent GIS database. Thus, a structural geological model was built with eight stratigraphically classified layers. In the northern part of the model area, no published borehole data were found at the beginning of the project. Therefore, the isolines of the bottoms of the stratigraphical layers and cross sections were used. For the generation of the structural model, the necessities of a numerical groundwater model had already been recognized, so that all of the layers were distributed over the entire model area. To obtain a hydrostratigraphically consistent model, the parameter distribution must be different from that of the purely stratigraphical model.

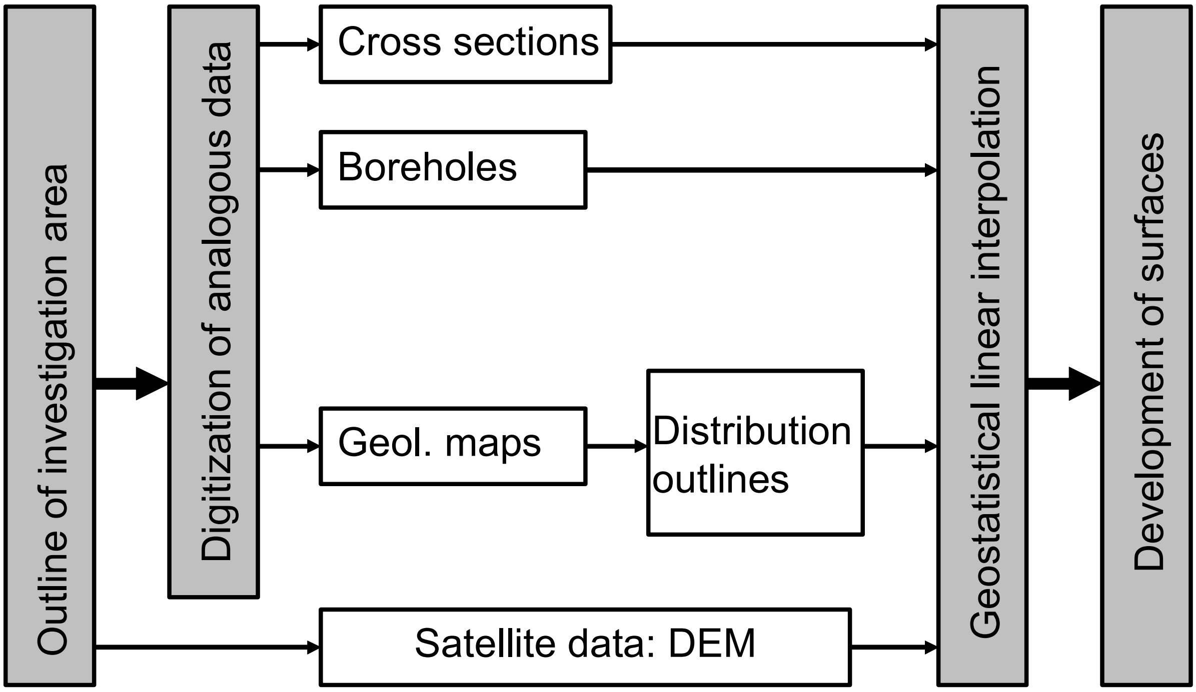


Figure 26: Workflow of the geological modeling for the Nubian Aquifer System.

The groundwater recharge was estimated very roughly and without a high spatial resolution, as described in GOSSEL ET AL. (2004). This procedure was used because there were several differences between this arid model area and model areas with humid conditions in the temperate climate zone. In this area, the precipitation is dominated by extreme storm water events with very long return intervals (>10 years). This cannot be compared to the recharge conditions in temperate climate zones under humid conditions. Additionally, there is a spatially and temporally varying registration of climatic data. In the valley of the river Nile, there are several stations with continuous registration over the last 100 to 200 years, whereas in the desert there are only widely distributed stations with short registration periods. The estimation of the recharge situation is bound to the model calibration and to several proxy data resulting from geological and geographical surveys. The very long investigation time (about 140000 years) was most important for the groundwater recharge estimation.

Based on the geology models and the very simplified groundwater recharge, a numerical groundwater model was developed. The workflow in Figure 27 shows that the numerical groundwater model was also simplified to a certain extent. The parameterization in this large area was carried out based on the database of a few hundred, often clustered, aquifer tests, and on the lithological descriptions of the geology (see Figure 28). A high resolution, as was used in the case studies of the subrosion valley Unterwerra and Untere Mulde/Fuhne, was not adequate for the modeling task in this case. Nevertheless, a three-dimensional model was developed to obtain results for the effects of climatic development on groundwater at different depths. The model was also used for additional research, e.g. regarding the genesis and stability of the saltwater – freshwater interface in the northern part of the model area. The effect of water level changes in the Mediterranean Sea on this interface was one of the main research topics. The boundary conditions for the numerical model are quite simple: In the west, south, and east, the basement outcrops are used as "no-flow boundaries". In the north the Mediterranean Sea and was used as an inner boundary condition and in the western part of the model area, the river Nile was modelled as a predefined head boundary condition (Dirichlet boundary condition).

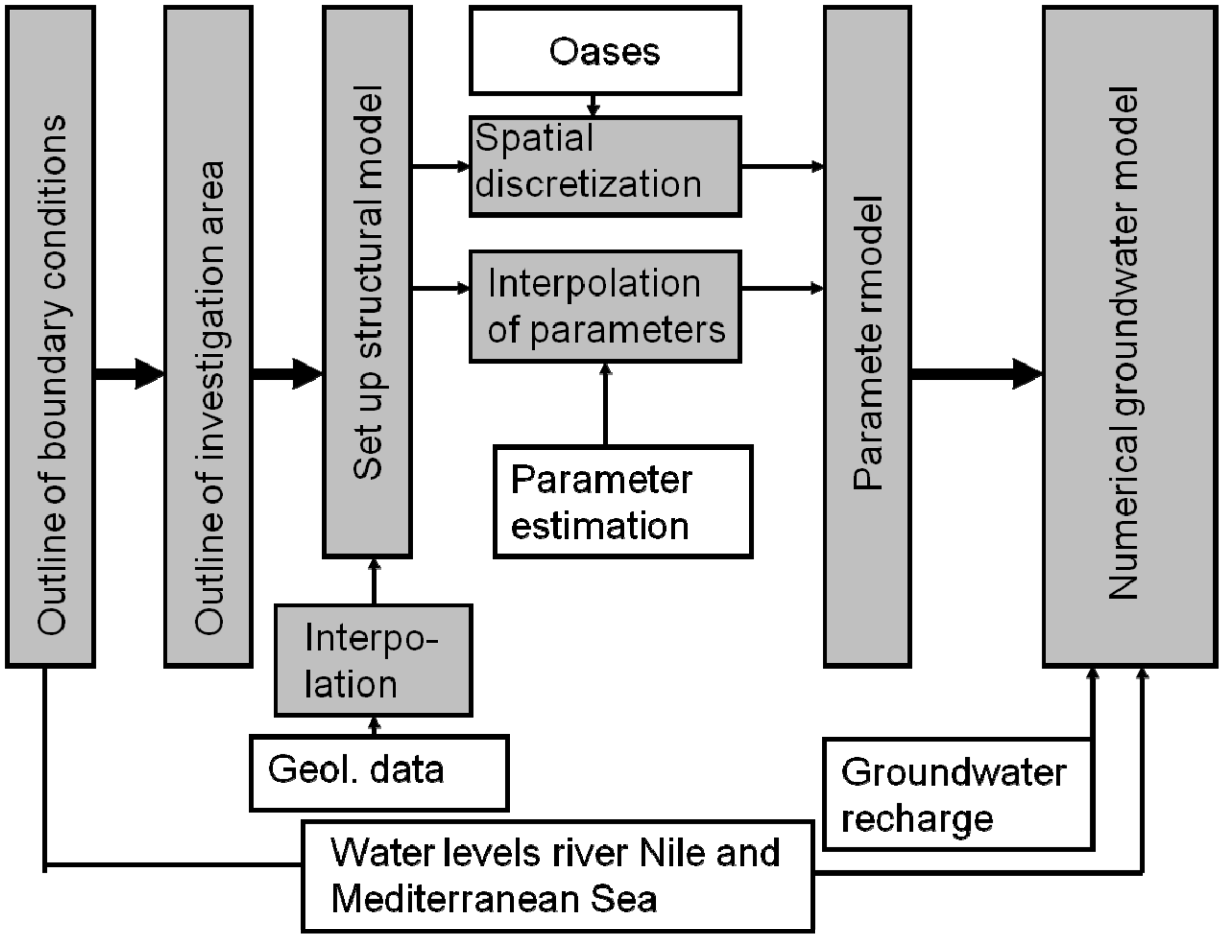


Figure 27: Workflow of the numerical groundwater modeling of the Nubian Aquifer System.

Connections to hydrological modeling systems were not implemented for the regional groundwater model. For the detailed models of Lake Nasser (SEFELNASR 2007), statistical methods for the hydrographs of the water level were used.

The coupling to the density-driven saltwater intrusion was first carried out with a higher horizontal resolution model at the Mediterranean Sea to ensure the stability of the model. In a second approach, the model was divided so that it was possible to enhance the vertical resolution.

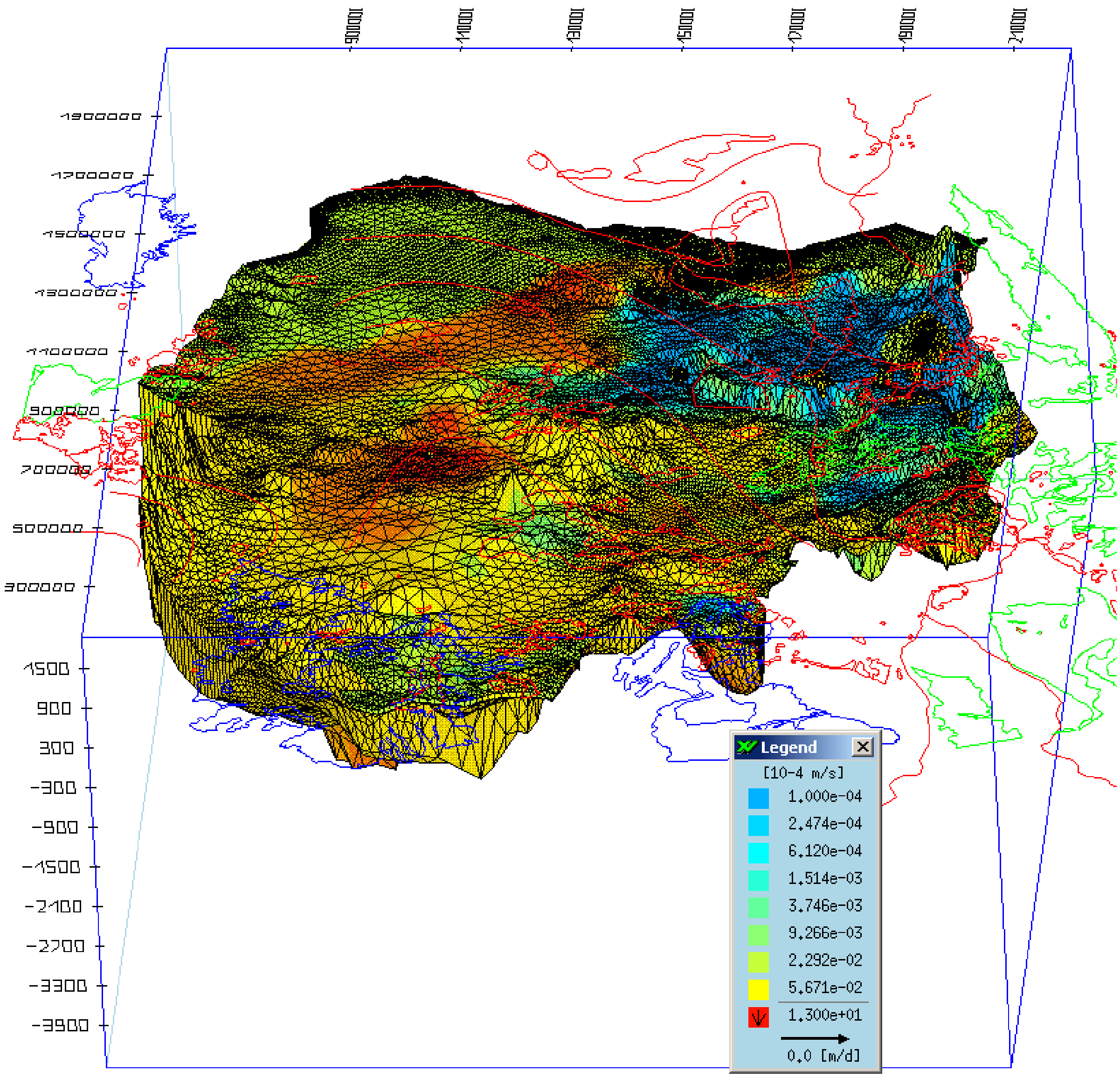


Figure 28: Hydrogeological structural model of the Nubian Aquifer System.

3.8.3 Untere Mulde/Fuhne

In the model area Untere Mulde/Fuhne, most of the described modeling systems were used. In this case study, a comparison of some modeling tools was possible. According to the structure of chapters 3.1 to 3.7, the single models for this area are described.

Geological models

In the Untere Mulde/Fuhne investigation area, several geological models with varying modeling systems and modeling tools were developed to obtain initial results for possible pathways and to outline and calculate the volumes of sorption capacities and of geological layers. The models were used in a scientific way to test the applicability of different modeling systems and modeling tools and to compare the results. FABRITIUS (2002) and WOLLMANN (2004) used constructive methods for two different subordinate areas, and HUBERT (2005) connected these two nearby areas and developed a model using statistical methods. These models have a very high resolution – 10 m for the investigation areas of FABRITIUS (2002) and WOLLMANN (2004) and 20 m for the model of HUBERT (2005). The modeling systems used by FABRITIUS (2002) and WOLLMANN

(2004) are based on constructive methods. Nevertheless, for visualization and data exchange, statistical methods support the modeler. The cross section-based construction, which takes 100 to 150 boreholes into account in both modeling areas, can cover only part of the total spatial extent of the model. For the area between the cross sections, statistical or geostatistical methods must be applied. In the modeling tools for these two modeling tasks, a complex triangulation that allowed the scientists to influence the mesh generation was used. The normally implemented Delaunay triangulation was first offered to the scientists, but this automatic mesh generation could be changed in a geologically meaningful way. The outline of a glacial channel or a gully erosion system was possible only with this algorithm because the boreholes encountered this system only a few times by chance. Without this feature, the boreholes beneath the channel would have led to an interruption of the flow path after the interpolation. The workflow of the geological modeling for this case study is presented in Figure 29. HUBERT (2005) demonstrated in detail that this result could not have been modeled (or could have been modelled only with great difficulty) through the use of automatic net generation and/or geostatistical methods.

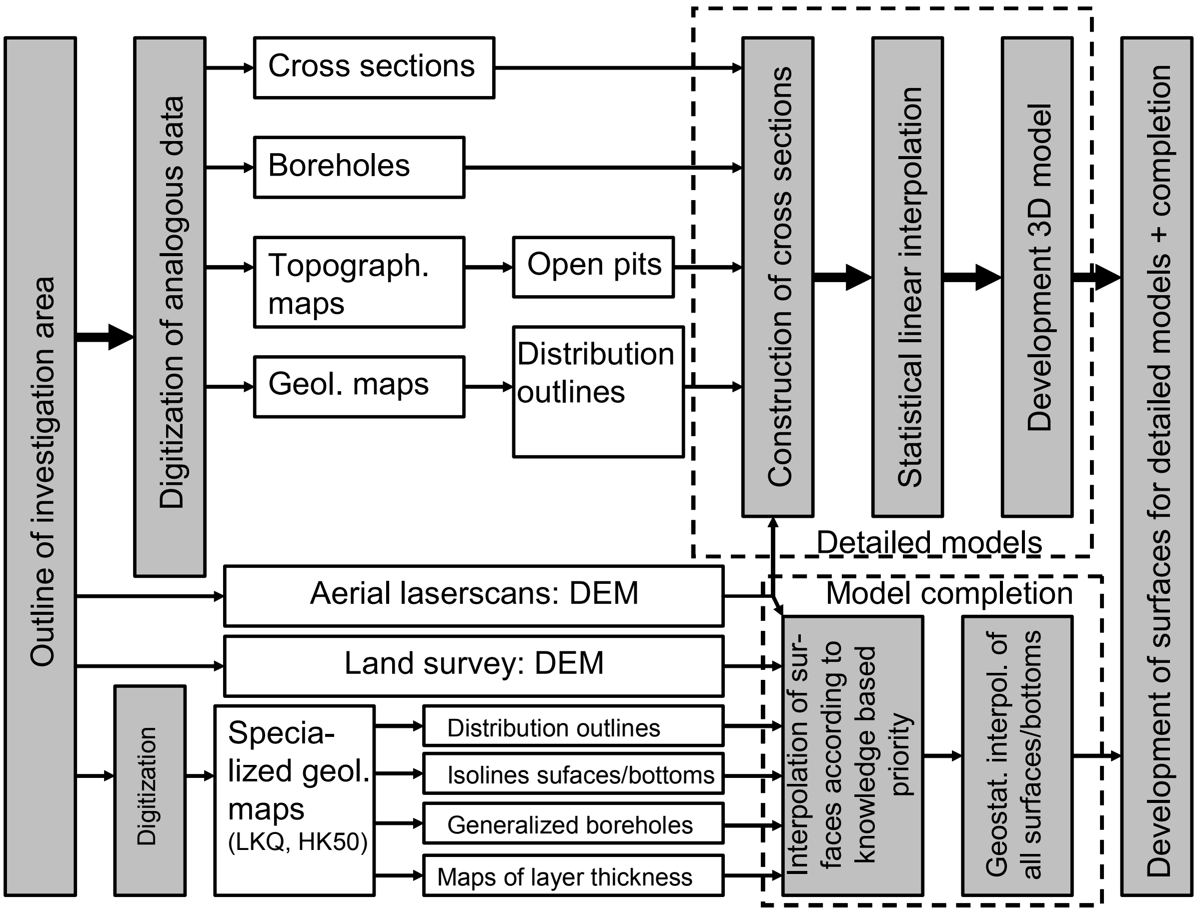


Figure 29: Workflow of the geological modeling in the investigation area Untere Mulde/Fuhne.

The pure stratigraphical orientation is characteristic of the geological model. The units with the most lithological differences were easy to classify; this was also true for the stratigraphical units, but additional rework was necessary for the hydrogeological modeling.

The development of a series of layers is a basic procedure in geological modeling. This series must be a consistent sequence of all the layers that should be modeled. With this “geological topology”, two main features are given implicitly:

1. Each borehole must be stratified seamlessly.

2. It is not possible to change this sequence (or it is possible only in precisely defined constellations).

Under these conditions, it is not easy to develop a model by matching lithological interfaces. Especially in the case of glaciofluviatile or glacial sands, a classification is very difficult, and thus a systematic modeling approach would be advantageous. Statistical methods can be a good preliminary stage for the refining constructive methods in these cases.

The complexity of the glacial horizons is superposed by more than 150 years of open pit mining activity. The impacts through all glacial layers and parts of the Tertiary layers (the coal layers have a topographical height of 30 to 50 m a.s.l., the ground surface is at 70 to 100 m a.s.l.) have led to very steep angles in the edges of the open pits. These anthropogenic geometries require very sophisticated models. (see Figure 30 and Figure 31).

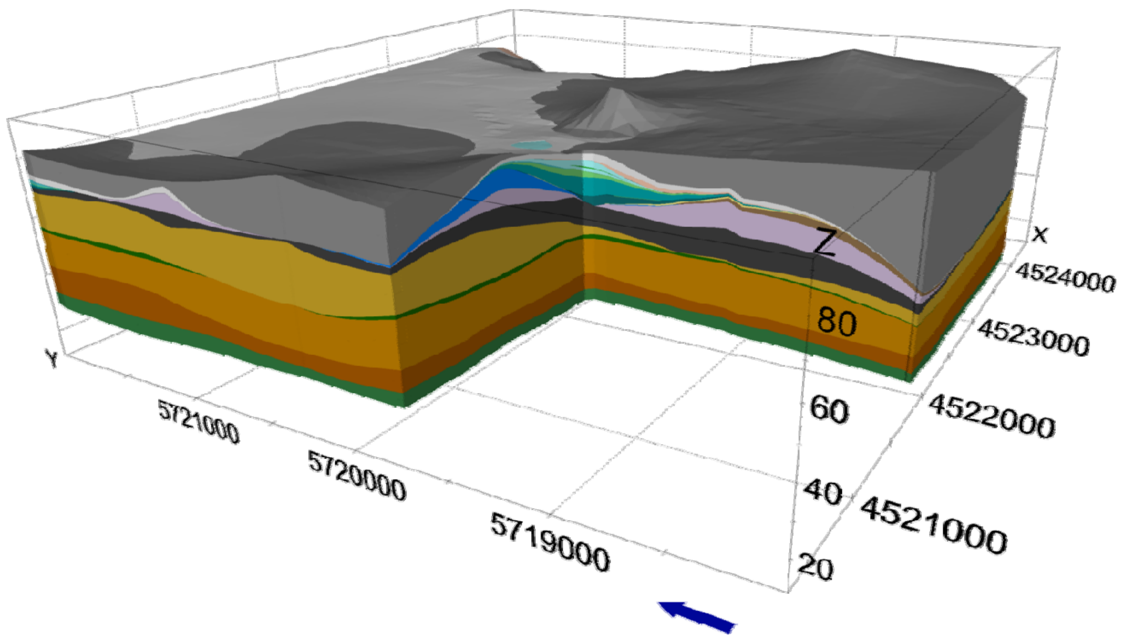


Figure 30: Geological model, developed with statistical methods. With only the database of boreholes, the resulting structures are too simplified. The interfaces of the geological and anthropogenic layers need to be corrected through additional geometrical operations. The main data for these corrections are the DEM and the horizontal and vertical dimensions of the open pit mines (HUBERT 2005).

The geological model demonstrates also the different potential applications of the diverse modeling methods. In the horizontally very continuous Tertiary layers with a litoral genesis, geostatistical methods are suitable for the interpolation of structures, and afterwards also for hydrogeological parameters. In the glacial sediments of the Quaternary, the structural heterogeneity cannot be represented by geostatistical methods. As shown in Figure 30 and Figure 31, there are obvious differences between the results of the statistical approach and of the constructive modeling technique.

The geological interfaces between the units from the Tertiary and the Quaternary can also be affected by geological processes, so that differentiated geostatistical analysis and interpolation become necessary. One example is the glacial channel from the Saalenian, which crosses the model area in a north-south direction.

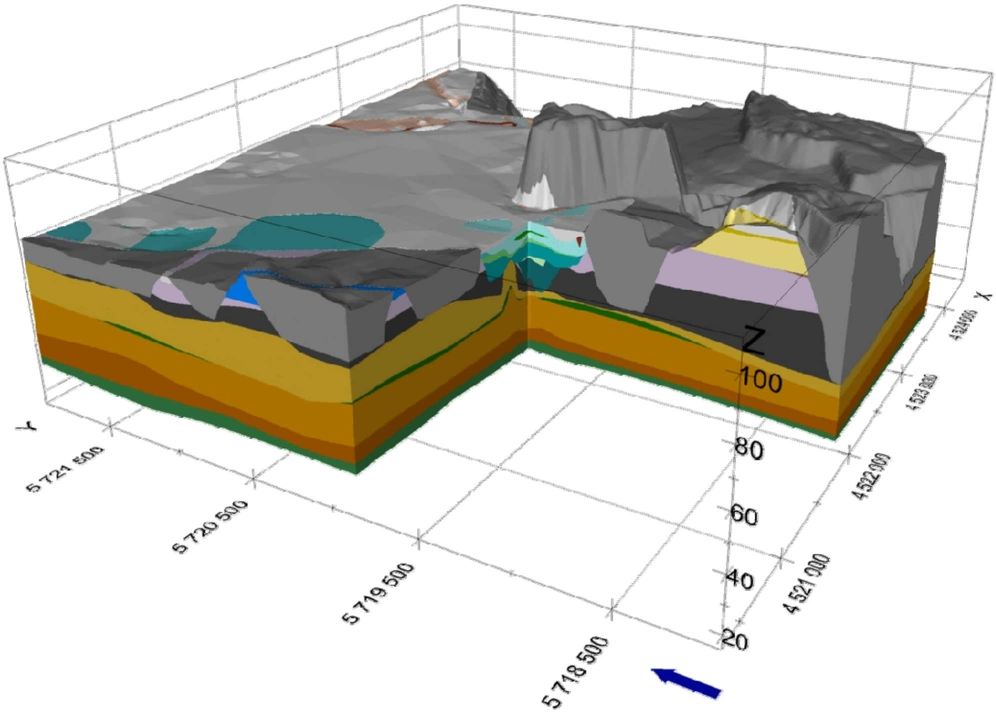


Figure 31: Geological model, developed with constructive methods. The triangulation for the interpolation of the bottom surfaces of the geological layers must be expertly adapted to the structures to adequately create the geological structures (HUBERT 2005).

Both modeling areas for the detailed geological modeling were placed in reference to each other. They were joined to obtain a homogeneous model of the central parts of the hydrogeological model. In this central area, the resolution of the hydrogeological model was set very high, according to the structural information and the points of interest. Owing to the necessities of solid boundary conditions for numerical groundwater flow and transport modeling, the hydrogeological model area had to be enlarged into a regional model area. For the areas outside the detailed models, the publicly available data sources of EIßMANN & MÜLLER (1978), MARCINKOWSKI & MÜLLER (1980), HELMERT (1984), and GROTE & KRÜGER (1984) were used. These maps are of widely variable quality, and they are not up to date; nevertheless they have to significant advantage: they were compiled by experienced hydrogeologists and they are (internally) consistent. A special procedure in compiling the data is necessary in order to use these maps for the modeling task and to reflect the differences in the reliability of the data. The harmonization of the geological units in the detail areas and the surrounding areas is the first step in the generation of the regional geological model. The structuring of the data was carried out mainly in a stratigraphical context in the maps of EIßMANN & MÜLLER (1978) and MARCINKOWSKI & MÜLLER (1980). The maps of HELMERT (1984) and GROTE & KRÜGER (1984) followed already a hydrogeological concept. The data of distribution maps, isoline maps for tops and bottoms of layers, values for layer thickness and – if available – borehole data in a generalized form were compiled in a GIS-based geodatabase. These data were classified according to their reliability and were handled in sequence with respect to this classification. The sequence of reliability was derived from the geological outline of the layers: layers with a lithology that was difficult to distinguish from the surrounding layers and with a low density of boreholes reaching the horizon received a lower priority as compared to layers without these demerits. From the regional geological model with its relatively low resolution, the area of the detailed models was clipped out and the data of these high-resolution models were inserted. This process is also described in chapter 4.7.3.

The use of the diverse modeling methods for the detailed modeling areas and the regional model demonstrated several systematic advantages and disadvantages of the modeling systems. One striking aspect is the possibility of updating models. In this area, many additional boreholes are being drilled and enhancement of the monitoring is still occurring so the updating capabilities are important. The geostatistically based modeling methods seem to have advantages with respect to this task. Structures of the already interpolated surfaces of the DEM and the outline of the mining areas will not change, so the cutting horizons can also be used after a recalculation of the geological layers. The adaptation of models with constructive methods takes more time because several cross sections need to be adjusted and the interpolation according to these new structures must be carried out again. Additionally, it would be very interesting if the dynamical hydrogeological model obtained a quasi-dynamical geological model to reflect the history of open pit mining in this area. This problem can be solved, with extensive efforts, using time slices in modeling systems, with statistical methods as well as in modeling systems with constructive methods. In this case, the geostatistical methods lose their advantage because the correction of the cutting features – the DEM and the outline of open pits – becomes very complex and time-consuming. For each new borehole in both cases, the geological model with all its layers must be created completely from scratch. For modeling with constructive methods, new cross sections that use the new information must be created. The adjacent cross sections require slight corrections and afterwards the model must be calculated again. The insertion of new facts is extremely problematic. Sometimes it is necessary even to go back to the bare input data of the boreholes and set up the whole model structure again. This can be very complex, and to some extent tedious and expensive. The modeling tools do not adequately support these features.

The history of open pit mining, for example, affects the possibility of using a quasi-dynamical geological model. Considering their static modeling concept, the recent modeling systems and the derived modeling tools are not able to solve such problems.

Modeling infiltration water

For the modeling of infiltration water, the most recent available method was used: In Gossel & Wycisk (2006), the first results of the method of TUB-BGR Wessolek et al. (2004) were described. The results of this modeling approach were compared to the values of Neumann & Wycisk (2003) and to the values from the method reported in Dörhöfer & Josopait (1980). Additionally, the runoff measurements of creeks and small rivers in the area, reported in Neumann & Wycisk (2006), were used for calibration. The base flow method was also applied to determine the infiltration rate.

The method of WESSOLEK ET AL. (2004) for calculating the actual evapotranspiration and the infiltration rate by subtracting it from the precipitation was applied according to the spatially distributed input data for the years 1840 to 2005. Because climatic data from a station inside the investigation area were only available for the period from 1947 to 1990 (DEUTSCHER WETTERDIENST DWD 2006), the dataset had to be elongated. Even for this period, data from several stations had to be used, but for the years from 1990 to 2005, published data from a station about 30 km away were inserted. For the earlier time span, a special procedure was employed because there were only data from Berlin, as reported in CHOWANIETZ & GOSSEL (1997). These data were correlated to the data of the Untere Mulde/Fuhne investigation area, and thus the dataset was completed. The potential evapotranspiration was calculated using the formula of TURC (1961), and the climatic water balance was calculated as the difference between the corrected precipitation values and potential evapotranspiration. Based on the calculation results of the actual evapotranspiration according to WESSOLEK ET AL. (2004) and of this potential evapotranspiration, a ratio for both was calculated for each year. According to monthly data of the potential evapotranspiration, a conversion to actual evapotranspiration was possible. With this procedure, several mistakes are made that involve the seasonal deviation from the yearly ratio:

- Differences in land use, especially on farmland, significantly influence the evapotranspiration. The crops cultivated over more than 160 years could not be reconstructed, and thus this factor must be ignore on account of the missing data.
- The depth to groundwater is also not constant. The groundwater extraction for open pit lignite mining has a significant impact. Additionally, there are seasonal variations, especially in regards to the yearly period of the evapotranspiration. For a first attempt, the recent depths to groundwater were used.
- The soil is significantly altered as a result of open pit mining. The distribution shown on the soil map (with a scale of 1: 25000) was nevertheless taken as constant because these changes and developments could not be reconstructed as well.
- Sealing of soils is a minor influence compared to the other factors reported above, but for this long time period it is not insignificant.

The consideration of seasonal factors in the empirical methods reported above and those discussed in DEUTSCHER VERBAND FÜR WASSERWIRTSCHAFT UND KULTURBAU (1996) is not possible. In this case, water balance and storage models for soils could be used in an enhanced modeling system. The modeling system described by HÖRMANN (2005) works with only four layers and would be advantageous. The missing data, especially for the land use history and the development of soils, lead to serious mistakes, even in an improved modeling method, so a detailed modeling approach would not be adequate for this area.

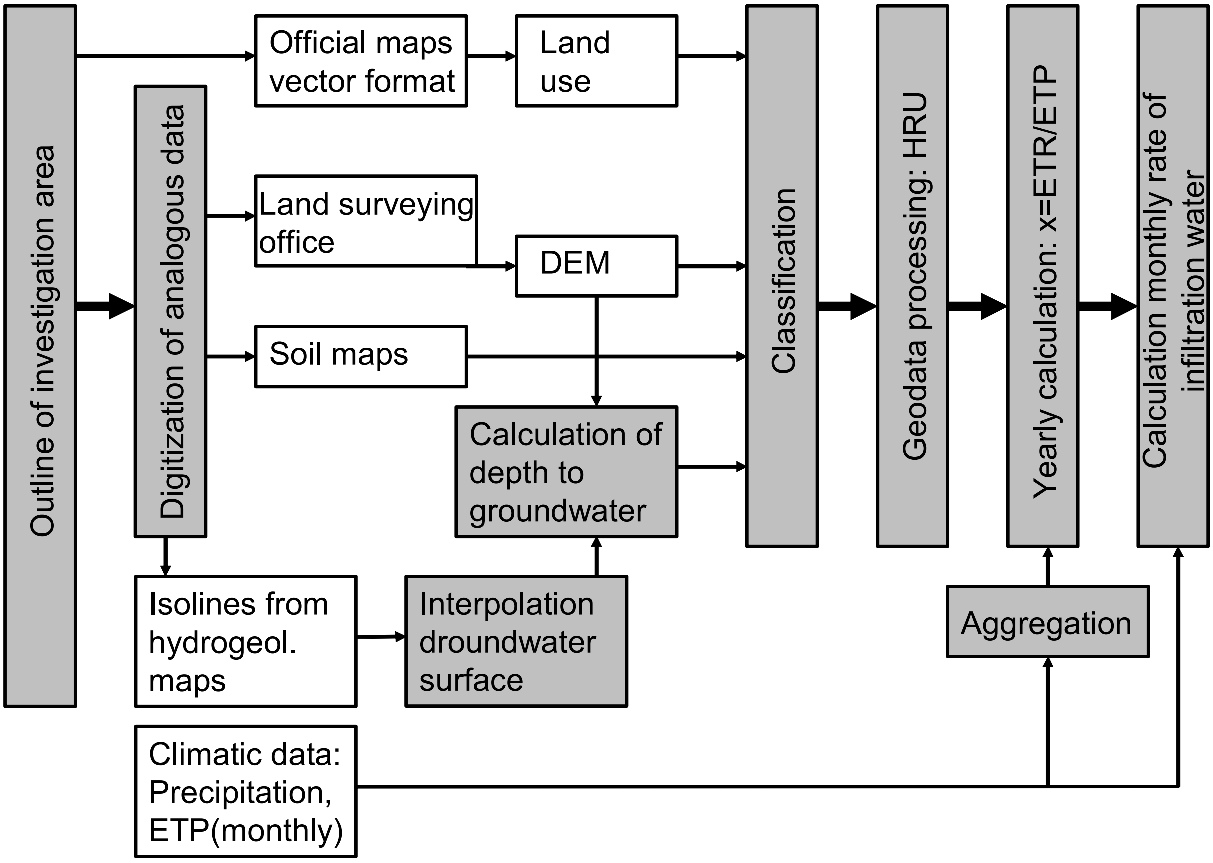


Figure 32: Workflow of the modeling of infiltration water for Untere Mulde/Fuhne.

For the application of these methods, GISs are very important. All the intersections of 2D geographical and hydrological data give the information for the hydrological response units. The functionality can be easily improved through programming. The soil parameters, land use parameters, and the classified depth to groundwater, as used by the modeling approach, were digitized from the respective maps. The overall workflow of the modeling of infiltration water is shown in Figure 32. The spatially distributed input data are shown in Figure 33 in several maps.

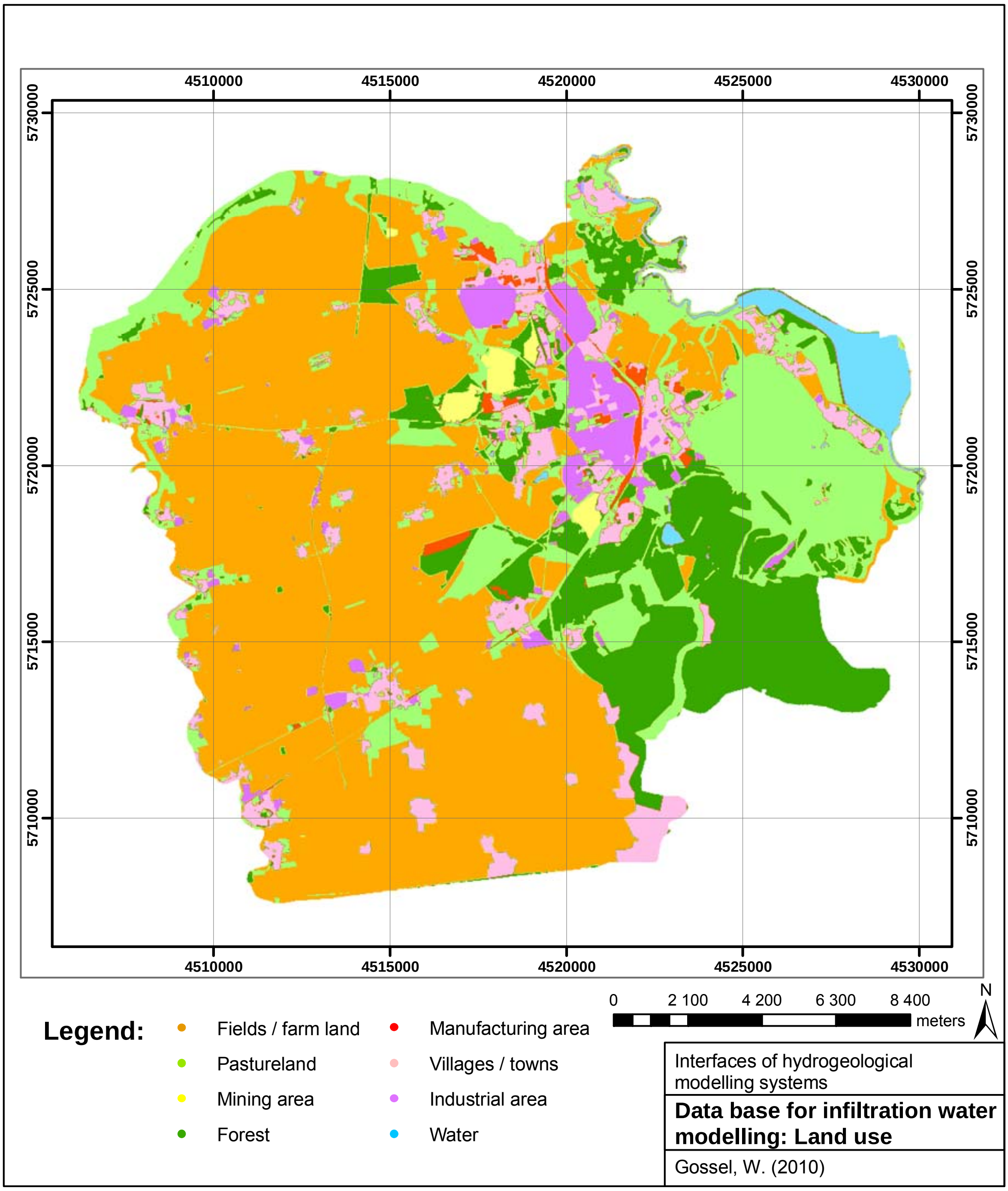


Figure 33: Spatial distribution of input data for the modeling of infiltration water in the modeling area Untere Mulde/Fuhne. The data for land use, soil and depth to groundwater were classified and processed to a 25 m raster.

A: Land use in the 1970s

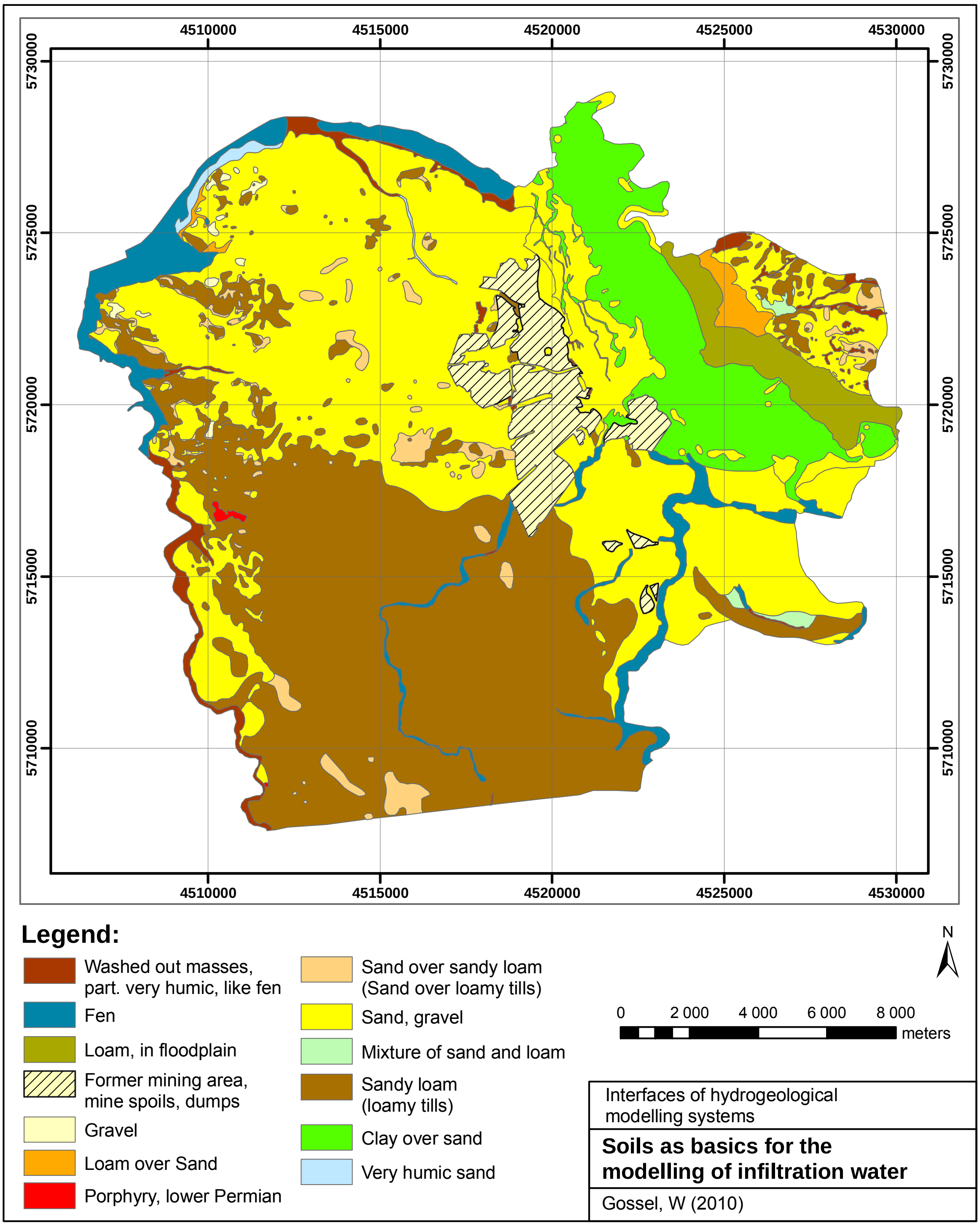


Figure 33: Spatial distribution of input data for the modeling of infiltration water in Untere Mulde/Fuhne. The data for land use, soil, and depth to groundwater were classified and processed to a 25 m raster.

B: Soil

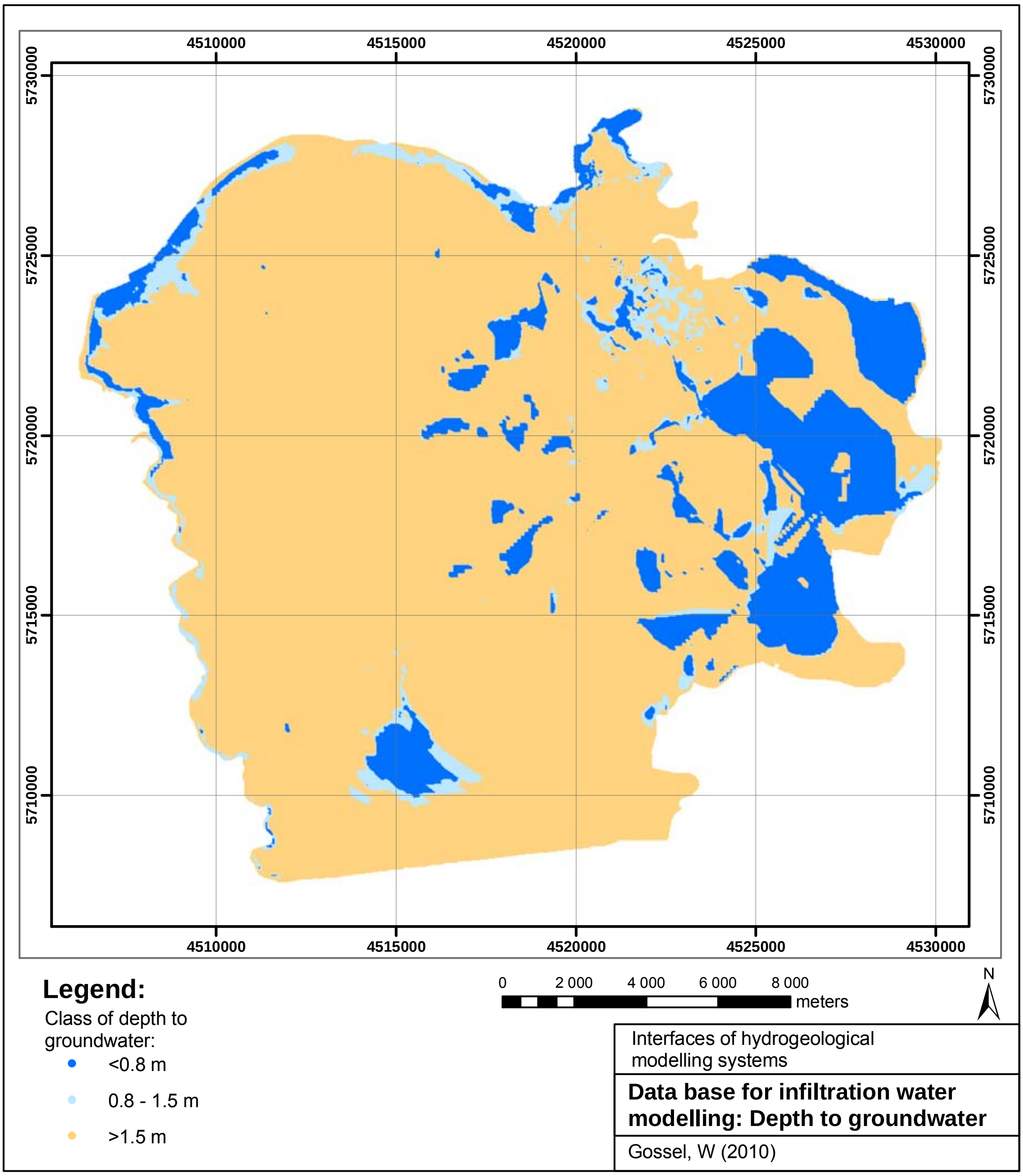


Figure 33: Spatial distribution of input data for the modeling of infiltration water in Untere Mulde/Fuhne. The data for land use, soil, and depth to groundwater were classified and processed to a 25 m raster.

C: Depth to groundwater

The average values and the values for a dry and a wet year for the rate of infiltration water are presented as examples in Figure 34 in its spatial distribution. In Figure 35 the time-dependent hydrograph is shown.

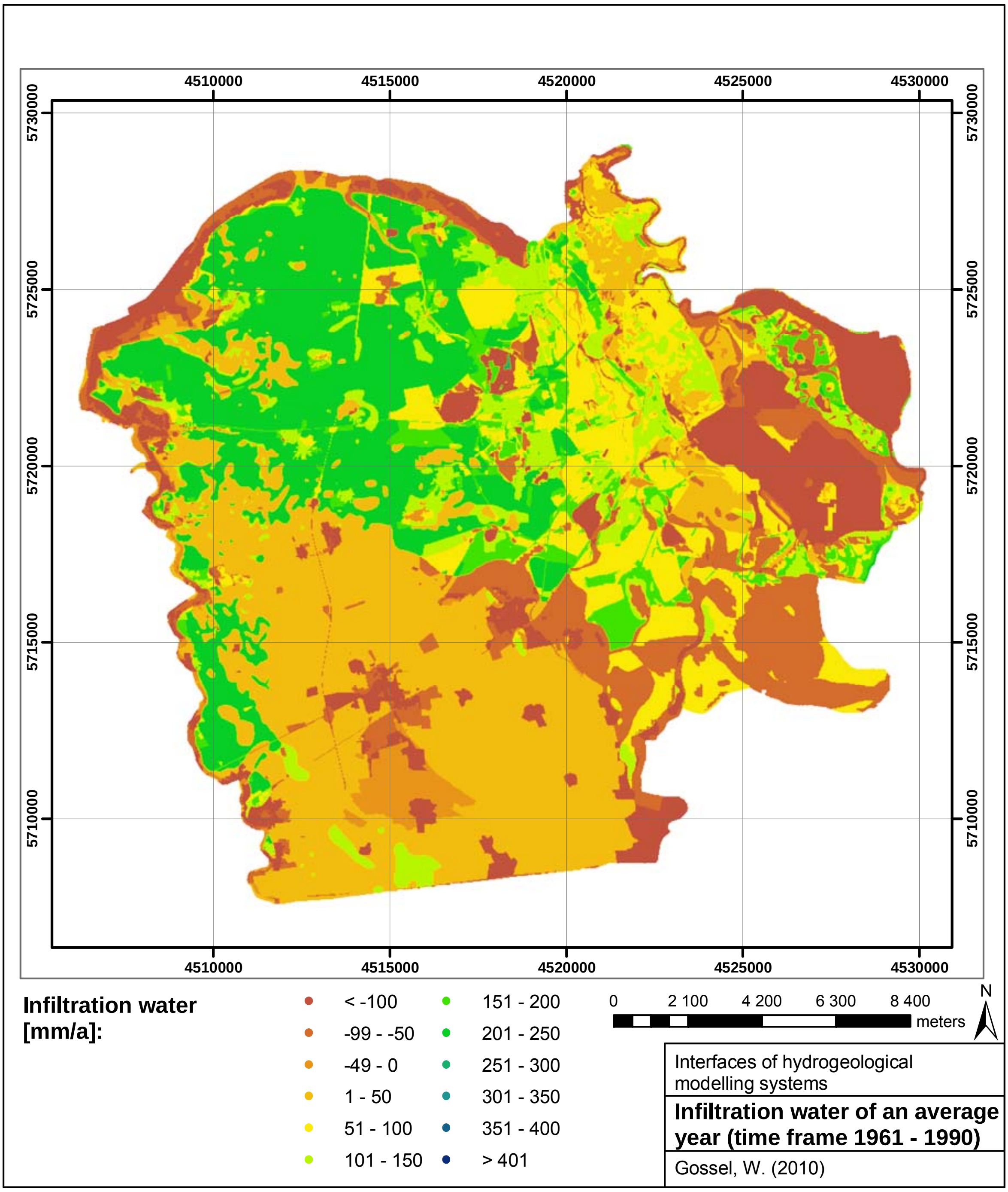


Figure 34: Spatial distribution of the yearly rate of infiltration water for a) an average year, b) a dry year, and c) a wet year. The calculation method of WESSOLEK ET AL. (2004) was modified for a higher temporal resolution with monthly values.

a) Average year from the period 1961 - 1990

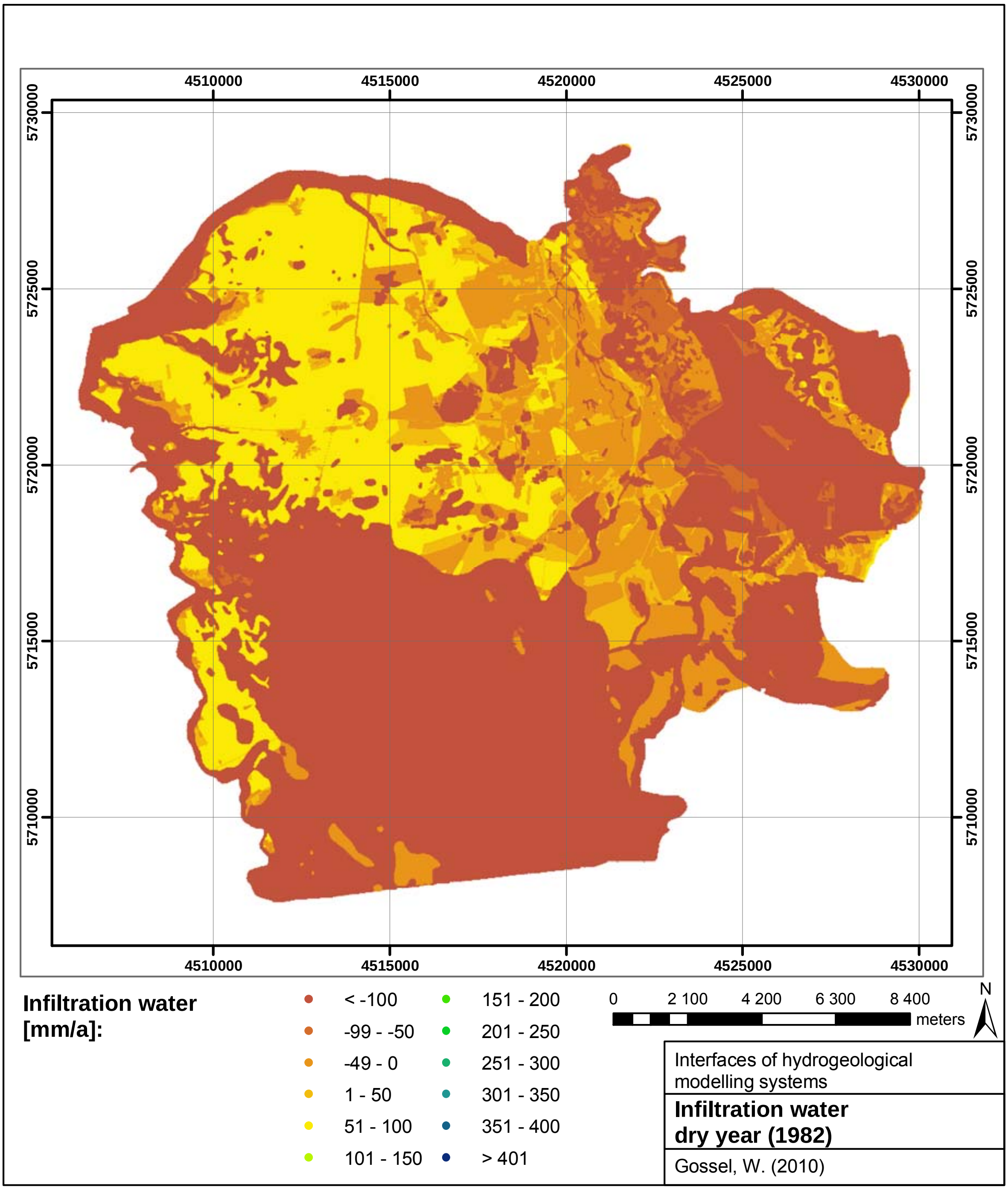


Figure 34: Spatial distribution of the yearly rate of infiltration water for a) an average year, b) a dry year, and c) a wet year. The calculation method of WESSOLEK ET AL. (2004) was modified for a higher temporal resolution with monthly values.

b) Dry year (1982)

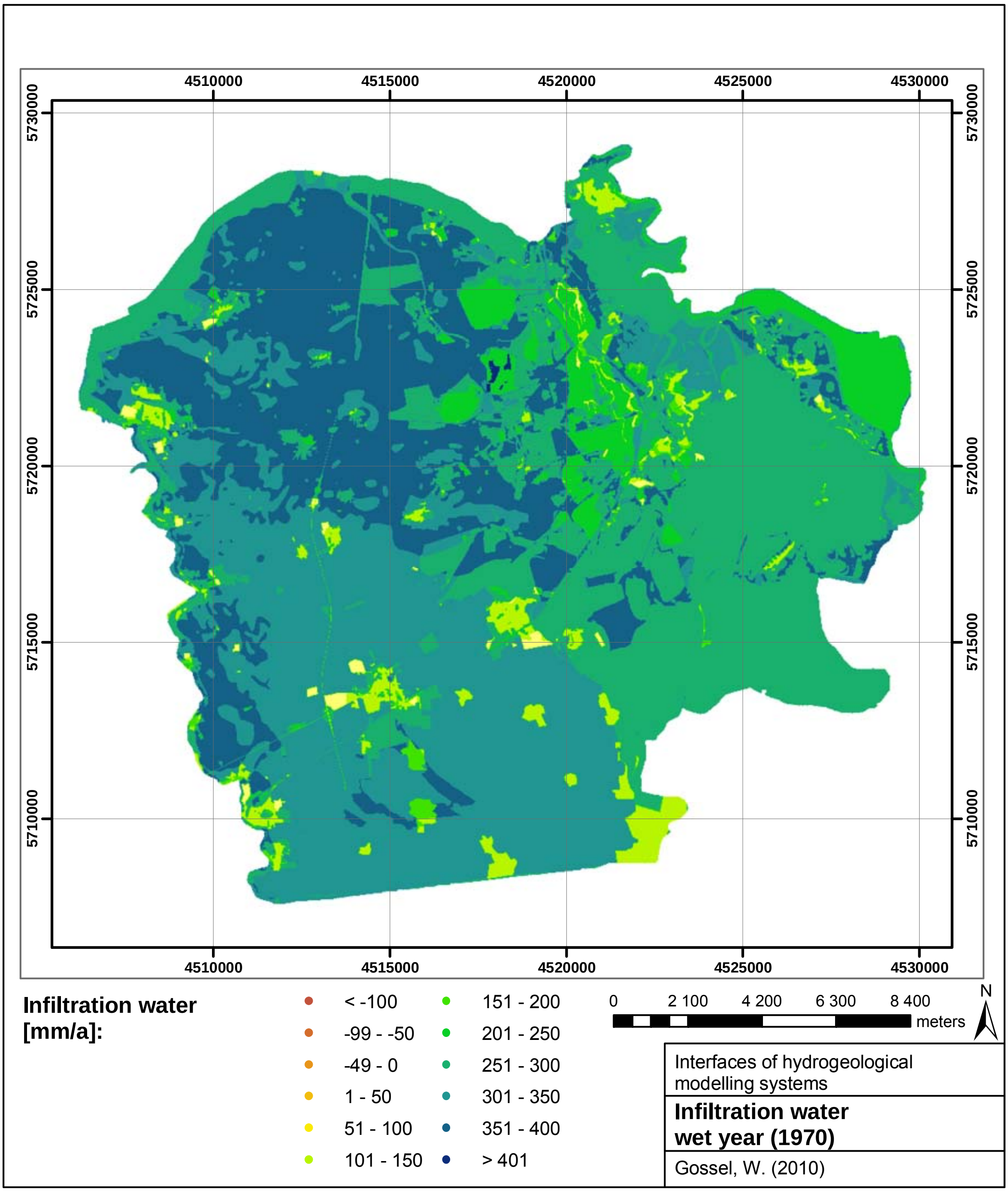


Figure 34: Spatial distribution of the yearly rate of infiltration water for a) an average year, b) a dry year, and c) a wet year. The calculation method of WESSOLEK ET AL. (2004) was modified for a higher temporal resolution with monthly values.

c) Wet year (1970)

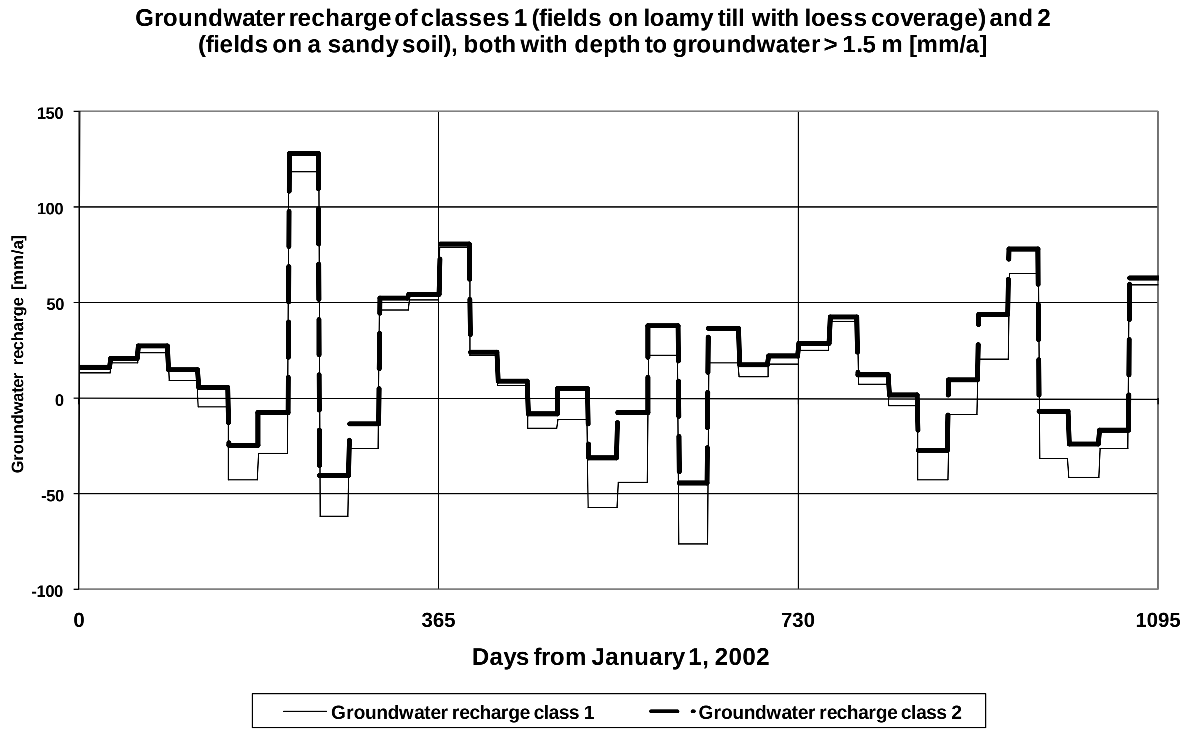


Figure 35: Hydrograph for the monthly rate of infiltration water of two hydrological response units for the years 2002 to 2004.

When analyzing the results, it is most important to see that – as is stated in CHOWANIETZ & GOSSEL (1997) and in NEUMANN (2005) – the temporal and spatial variability are of nearly the same range. Neglecting the temporal dimension by focussing only the average years of the whole observation period has to be seen very critical. The dynamic of the water balances cannot be adequately reflected by this reduction.

Modeling the unsaturated zone

The model of the unsaturated zone was coupled to the numerical groundwater model. Two different methods were applied for modeling the water balances in the unsaturated zone.

- The very simplified approach involving a retention time for the vertical flow through the unsaturated zone was applied quickly and effectively. The retention time was calculated for a "velocity" of 1 m per day. Only for areas with depth to groundwater > 30 m, relevant time shifts should be implemented on account of the 30 day temporal resolution of the numerical groundwater. These areas are very small.
- For the three-dimensional modeling of the unsaturated zone, the thickness and the structure of the geological model and the numerical groundwater flow model were adopted. The input parameters for this modeling approach with the approximation of the Mualem-van Genuchten function were taken from the numerical groundwater model. Only the initial conditions needed to be set. The coupling of the numerical groundwater model with the model of the unsaturated zone is presented in detail in chapter 3.

The small areas with a large thickness of the unsaturated zone were in negative correlation to the unstable behaviour of the model.

Numerical groundwater flow modeling

The investigation of interfaces in the form of a principle study is the primary objective of the numerical groundwater flow model for Untere Mulde/Fuhne. This includes testing and systematically investigating possibilities for a coupling of geological and hydrological modeling systems. The secondary objective is modeling the effects of the open pit lignite mining that has been occurring for over 150 years. The effects were assumed to be mainly related to the flow velocities in the southern part of the town of Bitterfeld. Considering these two objectives, a three-dimensional model is necessary. The workflow of the numerical groundwater modeling is shown in Figure 36.

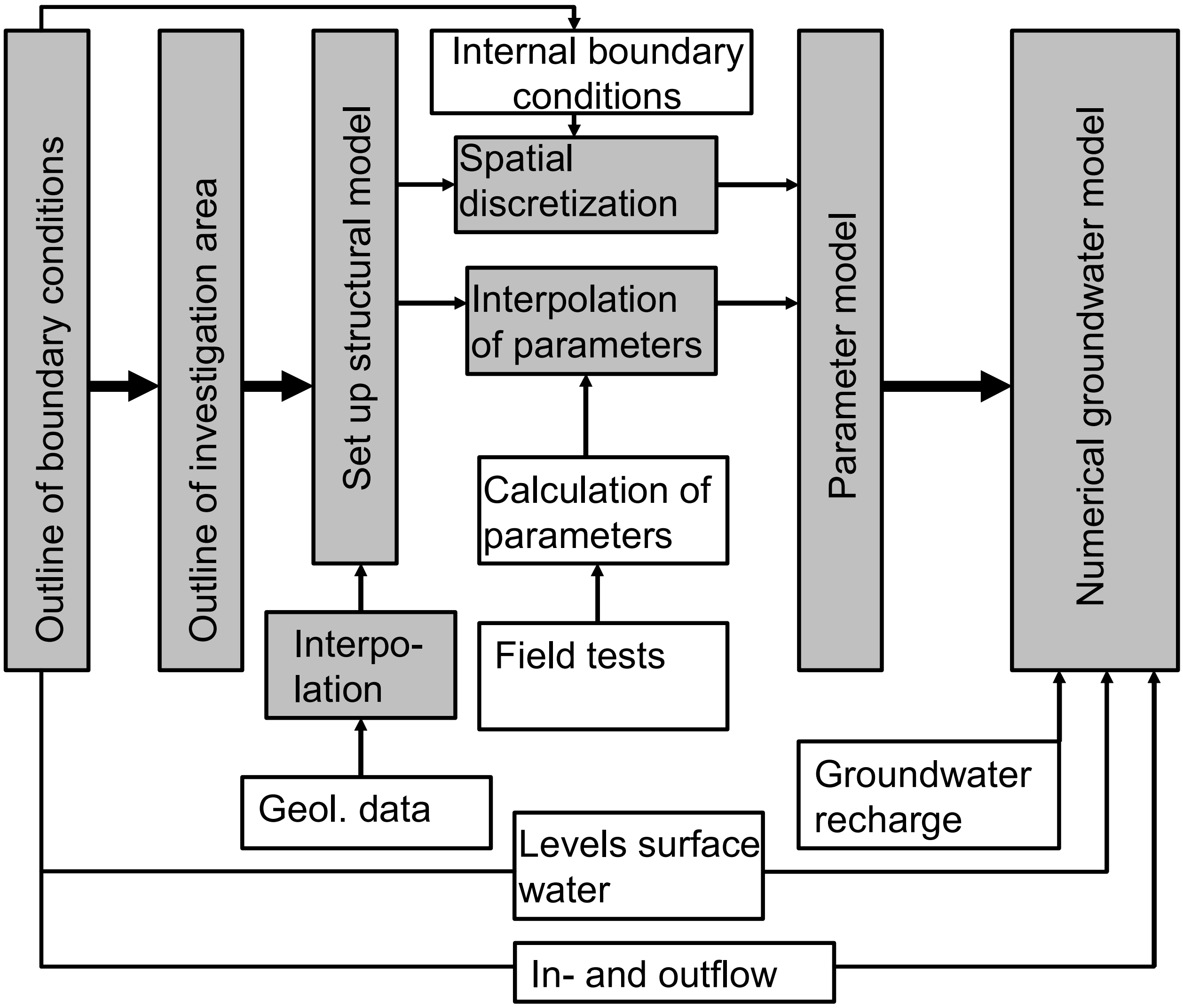


Figure 36: Workflow of the numerical groundwater modeling in the Untere Mulde/Fuhne investigation area.

The numerical groundwater flow model was set up as a finite element model based on the structures of the regional geological model with the insertions of the detailed models. For the spatial dimensioning, only hydrological boundary conditions were used. In the north, a creek, and in the east a large river could be used. In the west, the hydrological and geological boundaries meet because a small creek delineates the outcrop of hard rocks with very low hydraulic conductivity. The geological model must be adjusted in an adequate way because the geological model comprises geological lenses, channels, and fading out layers, especially in fluviatile, glacial, and periglacial sediments. These complex structures need to be converted to the numerical groundwater model without any information loss, though the layers must be preserved over the entire model area. Additionally, a parameterization according to stratigraphical units is not reasonable. The parameter distribution for groundwater models is oriented more to lithological units than to stratigraphical units. For this purpose, lithological borehole information was used in the detailed model areas. In the surrounding parts of the model area, the values were taken. For some parts, especially the deeper layers, assumptions based on the lithological description of geological units had to be made. In the mining areas, the layers were parameterized according to the description of the status quo because the historical data were only available in the form of a few topographical maps for a few time steps. The geometries of the layers had to be corrected in these areas on account of the steep angles at the edges of the mines to avoid numerical problems. To realize this in an accurate way, the structures were changed by being dragged through the mines, and afterwards, adequately adjusted parameterization was used according to the dumped material. In Figure 37 an overview of the regional groundwater model is shown.

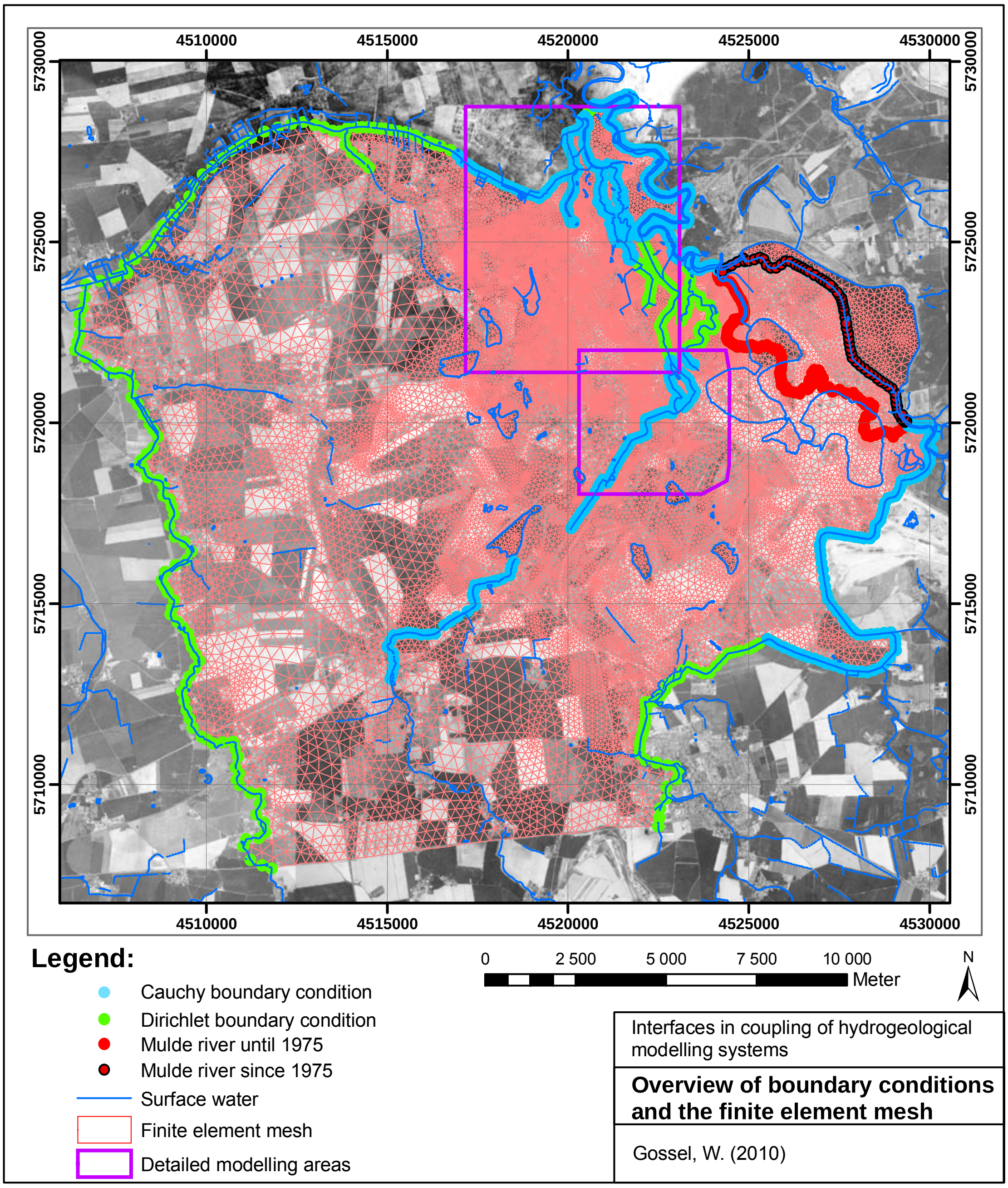


Figure 37: Overview of the regional numerical groundwater model. The basis is the finite element groundwater modeling system in which the horizontal discretization can be generated with large variations. The boundary conditions were defined in the north, east and west using time-dependent water levels (Dirichlet boundary condition), and in the south a watershed was used (von Neumann boundary condition). Additionally, the creeks with a definite connection to groundwater were defined as internal boundary conditions of a Dirichlet kind with a varying water level.

On the one hand, the groundwater recharge is of high importance for the water balances, and on the other hand it is of high importance as an input parameter for the numerical groundwater flow and transport modeling. It was adopted, according to the objectives of the modeling approach, with a high spatial resolution and a monthly time resolution.

For the Dirichlet-type boundary conditions, typical hydrographs of the creeks and rivers were generated on a statistical basis. They reflect the periodic flooding events of the river Mulde and of some tributary creeks in the northeastern part of the area. In the north and west, as well as in the southeast, a simple constant water level was defined because in these small, flat country creeks, no distinct flooding events are observed.

The model was divided into ten time shifts to reflect the development of the open pit mining and a postponement of the river Mulde at the end of 1975. The time slices are shown in Figure 38 together with these events. To realize this sequence, the water levels of the predecessor model must be set as the initial conditions for the next model. This procedure is responsible for a very long overall calculation time. The wells are very important for groundwater extraction in the mining areas. They were located directly in the mining areas, but the pumping rate was set only during the times in which the mine was active. As a starting point (1840), a steady state model without any effects from mining and with mean values of the water levels for the boundary conditions was chosen. The original paths of the river Mulde and of all the creeks that were registered in the maps of this time were implemented in this model.

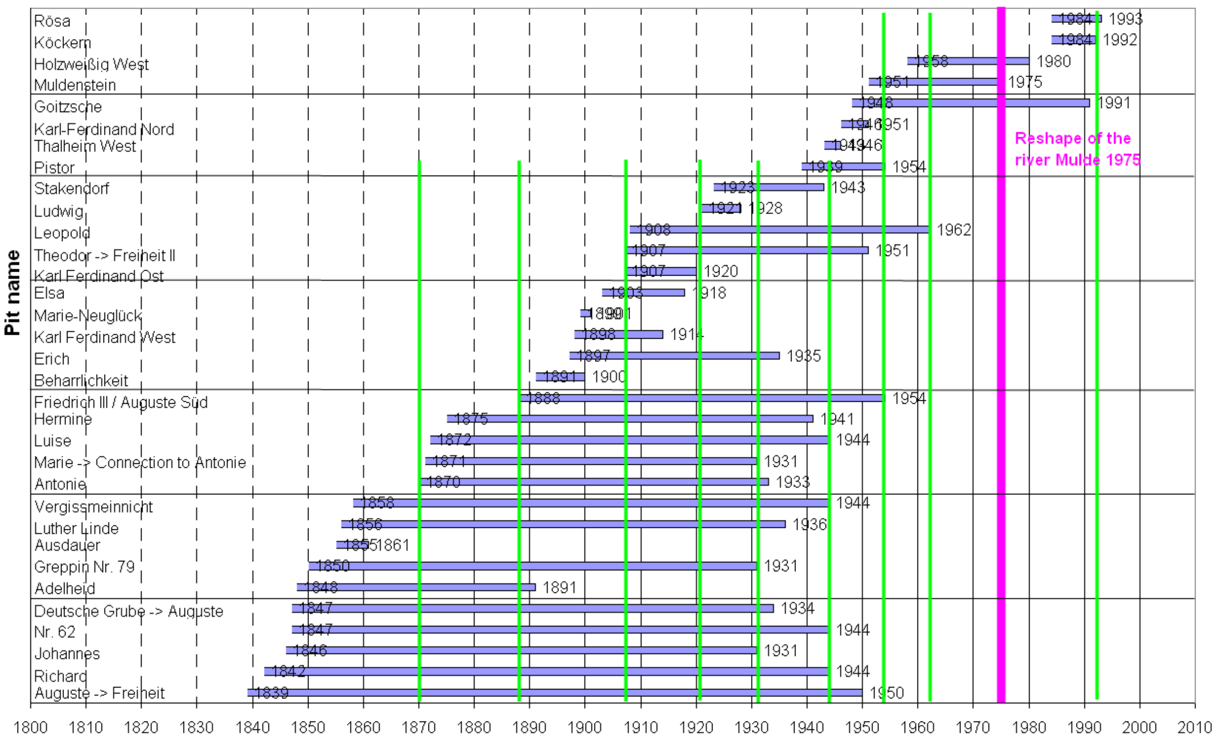
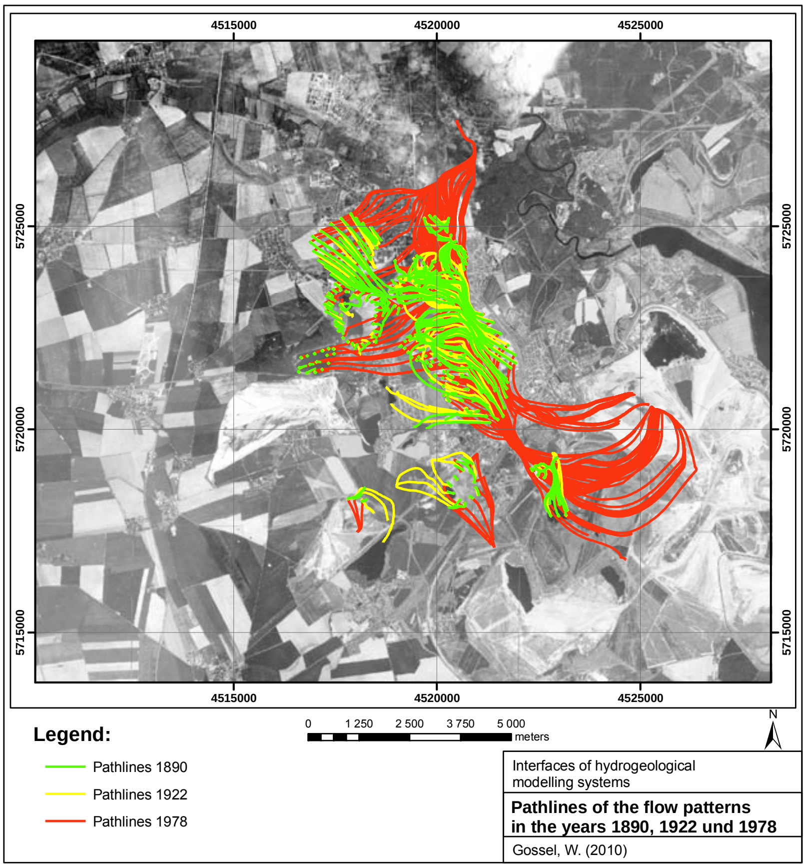


Figure 38: Development of open pit lignite mining in the region of Bitterfeld. The postponement of the river Mulde in the year 1975 was also a significant anthropogenic impact on the flow patterns of this area and is important for the numerical groundwater model, and therefore this time slice was also implemented. For each of the time slices, which are marked by green lines, a model was set up to optimally adjust the boundary conditions in the calibration.

The transition from the flow model to the transport model is the calculation of path lines. In this step, the three-dimensional directions of the flow of a representative elementary volume are calculated. These path lines were calculated in the steady state for reasons of simplicity and on account of the necessity of differentiating into distinct, time-separated models. Figure 39 clearly shows, for five time slices, the completely different flow regimes that result from groundwater extraction in the mining areas.



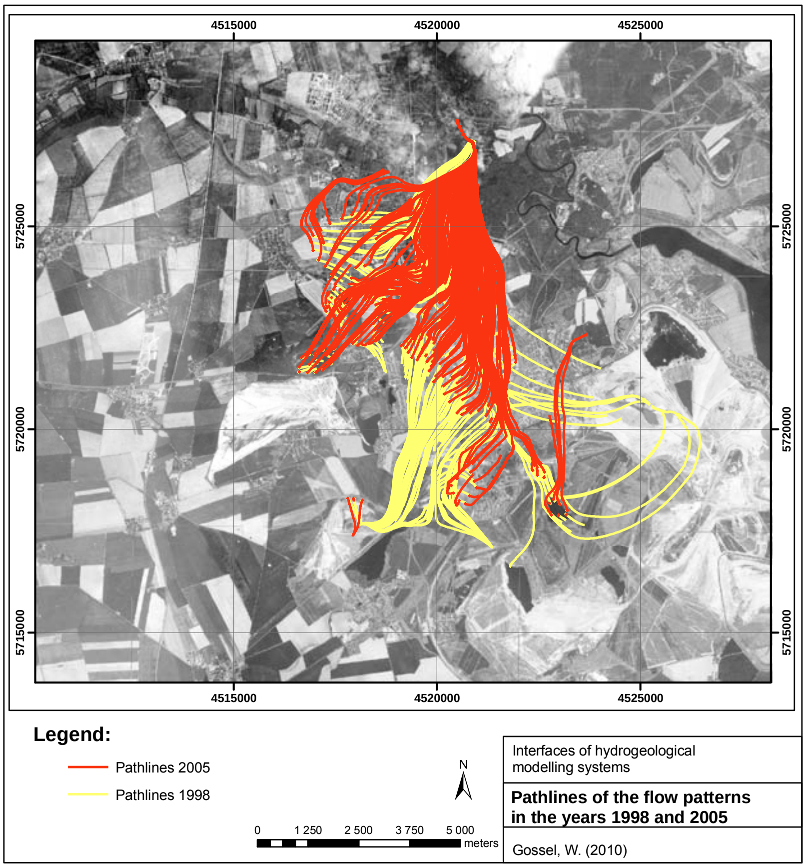


Figure 39: 2D-projection of the path lines for the flow regimes: a) 1890, 1922, and 1978; b) 1998 and 2005. The starting points were set at the same places for all time slices.

Modeling the deep depletion of groundwater levels and the increase after completion of the mining activity is challenging for most modeling tools. To avoid numerical instabilities in the rewetting of the cells after this serious depletion, several different strategies have been developed. One of these strategies is the adoption of the model structures during model operation and another strategy is filling the cells with only a small film of water. In both cases, the parameters of the model are maintained.

Numerical groundwater transport modeling

For the numerical groundwater transport model, the flow model was taken as the basis. The flow model was extended by the transport parameters of diffusion and dispersion and, in a second step, also by the sorption parameter. Modeling of biological degradation was not carried out because the database for the modeling parameters was not available. In addition, this is a study of principles study and is not meant to be a model for other effective or technical approaches. The usability of predictive modeling is therefore also very restricted.

The modeling approach without sorption reflects the behavior of the ideal tracer. The temporal succession and the special kind of discretization of the model lead to the transfer of model results from one time step to the next.

Hydrological model

The hydrological input factors were almost completely modeled with statistical methods in this area.

Precipitation

Monthly sums of rainfall were reported heterogeneously for several stations of the DWD (2005) for the period 1947 to 1990. From 1990 to 2005, daily measurements from a station only about 10 km away from the investigation area were publicly available (climatic station Schkeuditz, DEUTSCHER WETTERDIENST DWD 2007). To ensure the reliability of the datasets, they were correlated over a period of 20 years. The dataset for years prior to 1947 was the bigger problem. For the model area, no data were available. Therefore, the monthly data of the period 1947 to 1990 were correlated with the data from Berlin collected by CHOWANIETZ & GOSSEL (1997) (yearly sequences of the measurements during the years 1947 to 1990 of the Dahlem station, Free University of Berlin). The correlation coefficient indicated a very high congruence, so for the time 1850 to 1947, the “corrected” data from the Berlin station could be used for the calculation of the groundwater recharge. The mining in this area started in the year 1840. For the initial phase, the values measured from 1850 to 1860 were doubled.

Potential evapotranspiration

As described earlier, the potential evapotranspiration was calculated according to the method of TURC (1961). For this calculation, the datasets of the same climatic stations with the same procedures were used for the precipitation data.

Hydrograph of water levels of the river Mulde

The river Mulde is the dominant boundary condition in the east and northeast of the model area. Because its sources are in the mountains of the Erzgebirge, it has a very large dynamical influence, with high floods at the end of winter (snowmelt). Daily water levels were reported for the time range 1996 to 2005 (LHW 2005). A significant periodicity was generated from this hydrograph via a time series analysis, as is shown in Figure 40. The flooding effects were superimposed on this statistically based calculated hydrograph at the corresponding times in February/March. This statistically constructed time series for the yearly periodicity was taken for the entire modeling time on account of the missing data for the long period from 1840 to 1996. Of course, there are several arguments against this procedure:

- The characteristics of the catchment area have changed severely during this long period. The anthropogenic impacts on surface runoff have increased as a result of sealing.
- A closer connection to the climatic data was not followed because the correlation to the runoff of a river coming from mountains about 150 km away from the investigation area was not significant.
- The runoff behavior changed during this long period, also as a result of water engineering.

Despite these doubts concerning the validity of the model assumptions, there is good agreement between the measurements and the results of the model. Additionally, the dynamical behavior of the creeks in the northeast section of the area can be attributed to the infiltration of water from the river Mulde via the Weichselian gravels. A flow back need not be assumed. This dynamic of the river Mulde affects only some of the creeks. Other creeks are not influenced by floods.

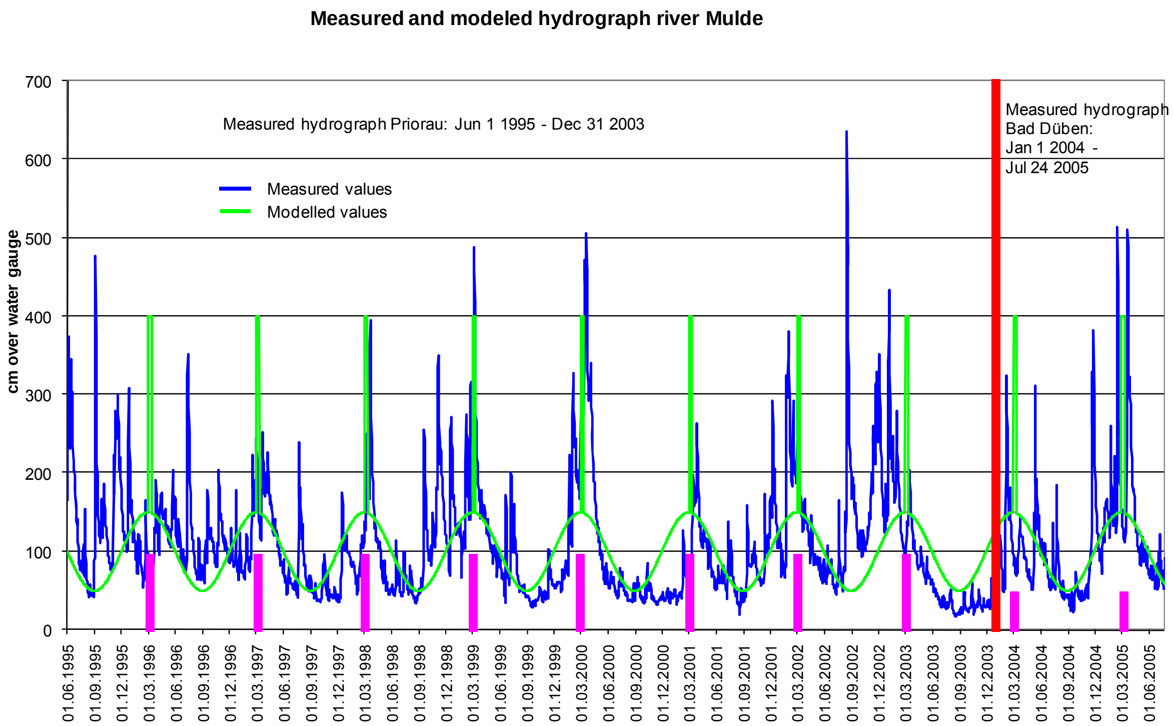


Figure 40: Hydrograph of the water levels of the river Mulde. The comparison between measured values and the statistically modeled time series of water levels exhibits an overall accordance of the values. In a detailed analysis, there are several deviations. The purple lines are set for the stages of the annual floods in March. The correlation coefficient of the time series of 3707 measured and modeled values is 0.31 and thus fulfills the requirements for a significance of 99%.

Runoff of several creeks in the northeast of the model area

In the context of a research project, the runoff and the contamination by certain substances of several creeks in the model area were measured in the period of February 2005 to April 2006. The measurements were carried out every two weeks to identify the dynamical behavior of the exfiltration of these substances to the surface water (NEUMANN & WYCISK 2006). These measurements enabled the modeling of the boundary conditions in this part of the model area, and they revealed the dependencies between the river Mulde and these creeks. A real modeling of surface water runoff based on the Navier-Stokes equation was not carried out.

Modeling in environmental geology

In this model area, numerous investigations in environmental geology have been carried out (WEIß ET AL. 2002). The research focused on the investigation of contamination and remediation but modeling was not on the agenda. Thus, the following passages do not take these investigations into consideration.

For the statistical investigations of THIEKEN (2001), special statistical tools were used, just as in other scientific disciplines. Factor and cluster analysis are widespread, and they enabled very detailed results for several research topics. The Hasse diagram technique, shown in BRÜGGEMANN ET AL. (1999), facilitated the classification and ordering of hazardous substances and regional distributions.

The physicochemical and chemical groundwater parameters, provided by RICHTER (2003) and RICHTER ET AL. (2004), were interpolated in 2.5D with standard tools in geostatistics, based on a solid data analysis. In contrast to WYCISK & GRATHWOHL (2005), no real 3D interpolation methods were applied. The differentiation according to hydrostratigraphical criteria was derived from the structures of the geological models. Thus, distributions were calculated for both dominating aquifers. Additionally, for the investigation of anomalies of the groundwater temperature, the geothermal gradients were regarded in the model calculations as an example. The interpolation of contaminants from the reports of WYCISK & GRATHWOHL (2005) was a first step toward real 3D distributions. These interpolations were based on sophisticated geostatistical software but did not consider hydrogeological structures and hydrodynamical parameters.

3.8.4 Examples for the implementation of modeling systems in tools

The modeling systems are actually implemented numerous tools. The tools presented in the following chapters were applied only for exemplary models. The presentation cannot be an assessment of modeling systems applied to solutions of very specific tasks, for several reasons:

1. The tools are changing rapidly. Nearly every year, additional features are created. The tools may be completely revised, or they may stop supporting old data formats or features. This rapid and fundamental change would lead to a bad decisions or incorrect assessments, which would suit neither the tools nor this work.
2. The number of tools with specific features has become very large and this is an advantage for the users. Several tools have evolved as “market leaders“, but the most innovative and adjustable tools are open source tools. Several tools were developed with very specific methods to solve a wide variety of

technical problems, also, regarding the direct modeling task, they were intended to quickly improve the modeling process. Therefore, an assessment of a subset of these tools would not fulfill the requirements of this extensive variety.

3. It is nearly impossible to change from one tool to the next, even with standard tools like GISs. Testing and training for these tools require several months or even several years because they are very complex and specific. Thus, a comparison will merely reveal the weaknesses and preferences of the scientist in solving specific problems – it will not indicate the advantages and disadvantages of the modeling tool itself. In case of open source software, there is a question not only of the availability of functionality and methods but also of the ability of the scientist to implement additional functionality. Current commercial tools have successive programming interfaces for the implementation of new functionality.

For these reasons, only a few tools are mentioned here, these were applied to the case studies and used to generate the possible solutions. In the case of highly specialized scientific problems, the scientist should feel encouraged to develop new properties, methods, and interfaces for the available tools.

In addition to several open source GISs – i.e., QuantumGIS©, SAGA© and GRASS© - the tools from ESRI®, especially ArcView® but also ARC/INFO®, were used. For ArcView® 9.x alone, approximately 1000 VBA scripts are presented by users on the ESRI servers. Each of them is a specific add-on for diverse purposes. For the scripting language of ArcView® 3.x, Avenue, a comparable number is available. The documentation of these scripts is sometimes a bit sparse, but in most cases, additional information is found in the comments of the scripts. Single tasks can be solved easily by scripts - the alternative is the own programming via defined interfaces. One disadvantage of the ESRI® tools is that they are intended for handling areal data and thus are not suitable for three-dimensional geological modeling. However, the data can be exchanged in both directions with geological modeling tools, so an integrative approach can be realized.

For the numerical groundwater modeling mainly the tools Visual Modflow® (WATERLOO HYDROGEOLOGIC 2002, a pre- and postprocessor of the free kernel MODFLOW© (USGS 2000)) and Feflow® (WASY GMBH 2005) were applied.

The geological modeling was carried out with the tools GeoObject 2® (INSIGHT GEOLOGISCHE SOFTWARESYSTEME GMBH 1998), GSI3D (LITHOSPHERE GMBH 2006) and EVS/MVS® (CTECH INC. 2006), but for several modeling tasks the capabilities for the visualization of the interpolation tools and of GISs are adequate.

In the hydrological context the modeling of infiltration water was completely implemented through the own resources via VB®, VBA®, and C or C++ programming. The surface water “modules“ were also written for this modeling task because statistical methods were needed, rather than the more complex modeling methods of numerical runoff.

For the unsaturated zone, both kinds of methods were applied: Simple modules were written, mostly for very specialized tasks; for the more complex tasks and for a comparison with the results of the simple methods, standard tools such as the WHI Unsat-Suite® (WATERLOO HYDROGEOLOGIC 2002) and Hydrus1D© (SIMUNEK ET AL. 2005) were applied.

Modeling in environmental geology was supported only in exceptional cases by standard tools such as RBCA (RBCA Toolkit for chemical releases, GSI ENVIRONMENTAL, 2007), RAM (Risk Assessment Model, ESI ENVIRONMENTAL SIMULATIONS INTERNATIONAL LTD, 2005) or RISC (RISC4, ESI Environmental Simulations International Ltd, 2002). In most cases, standard GIS tools with only a few improvements and extensions were sufficient for these tasks.

3.9 Summary of modeling systems

The hydrogeological modeling systems investigated in the context of this work were extended into several disciplines: geological modeling, infiltration water modeling, unsaturated zone modeling, and flow modeling for the saturated zone were the main stages in this approach. Transport modeling, hydrological modeling, and modeling for environmental geology were only used by chance and when necessary. The available data sources and input parameters must be adapted to each other. This is supported by numerous modeling systems. Deterministic modeling methods were preferred because the structural validity and the behavioral validity are normally satisfied in these tools, whereas this cannot be guaranteed when using statistical tools. In regards to coupling modeling systems, it is important to see which methods are applied, because the results of the statistical methods have, in most cases, the advantage of a higher flexibility as compared to the constructive methods.

In the case studies, different modeling systems were applied according to the modeling tasks. Figure 41 presents an overview of the employed methods.

Modelling system, compartment	Geology	Infiltration water	Unsaturated zone	Groundwater	Hydrology
Model area					
Subrosion valley Unterwerra	constructive	empirical	-	Finite Elements	statistical and constructive
Nubian Aquifer System	geostatistical	statistical	-	Finite Elements	statistical and constructive
Untere Mulde/Fuhne	constructive and geostatistical	empirical	(Finite Elements)	Finite Elements	statistical

Figure 41: Application of modeling systems and methods in the case studies.

For the geological modeling, the systems based on statistical and descriptive methods were preferred, whereas the empirical methods met the needs of infiltration water modeling. The unsaturated zone needed to be modeled only in one case study. The application of empirical and numerical methods was tested in this study. In the saturated zone, deterministic numerical methods are dominant for flow modeling as well as for transport modeling. Hydrological model data have been considered only via statistical modeling.

4 Interactions of hydrogeological modeling systems

In chapter 3, the modeling systems, the data needed for setting up a model and the methodical basics were described in detail. The case studies presented in chapter 3.8 show that the application of each modeling system led to improved analyses and to a clarification of theoretical and practical problems. The descriptions of the workflows demonstrate that these procedures are very complex and sometimes time consuming. Hydrogeological modeling systems are therefore used mostly as standalone tools because they are highly specialized, and for each model some initial training is needed. This task of connecting hydrogeological modeling systems is bound to the consideration of the different compartments. Nevertheless, the solutions with interactions between adjacent modeling systems are readily apparent. When this interaction is built through a transfer of boundary conditions or parameters, the modeling procedure is not very complex. Although there might be numerous datasets, the number of different parameters or boundary conditions is usually manageable. In a real coupling of modeling systems, the complexity increases. This leads to the question of an adequate solution to a hydrogeological problem. Whereas HILL (2006) stresses the necessity of simple or simplified solutions and therefore also the application of the most simple modeling systems and tools, GOMEZ-HERNANDES (2006) points out that there is great potential for the development of models with higher complexity if they are closer to reality. This statement is restricted to certain steps in the numerical hydrogeological modeling process. The point of view of this question is important in regards to the phase of development of a conceptual model, and it can easily be pushed into the corner of philosophical considerations. The further workflow and the choice and application of diverse modeling systems depend on this decision. Both lines of development of complex interactions between modeling systems should be considered in detail. The definition of complexity creates several initial problems: SEPPELT (2003) derives the complexity from four factors:

1. The system must be open thermodynamically.
2. Diverse components must be included. The modeling systems should include different compartments, but one can also connect modeling systems for a single compartment, e.g. in relation to groundwater for flow and transport modeling.
3. The connections of modeling systems must be non-linear.
4. The heterogeneity must be high in the spatial and temporal dimensions.

HILL (2006) quantifies complexity according to the diversity and number of parameters and boundary conditions that need to be considered in the modeling approach.

For GOMEZ-HERNANDES (2006), the central criteria for the quantification of complexity are indefiniteness and the uncertainty of parameters and boundary conditions.

The question of complexity is evident in the problem definition and solution, and it should be considered by including new working techniques in the context of the various capabilities of the hydrogeological modeling systems that are currently available.

The definition of modeling given in chapter 1.2 points out that at the starting point, detailed and comprehensive descriptions of the modeling purpose and the processes to be modeled should be given. The availability of verified modeling tools – i.e., tools that are proven for the correct implementation of the formulated basics and for a wide range of processes – supports this task. “Toolsets” are available for processes that are not implemented in modeling tools. This helps to complete the demands of the modeling approach (SEPPELT 2003). This procedure is characteristic of today's applied research. For fundamental scientific questions, the purpose of the modeling is not well defined in advance owing to the overall nature of research approaches. A result cannot be anticipated in these cases. For an applied and task-oriented model other modeling techniques can be applied. In these case studies, the questions of complexity and interactions of modeling systems in a modeling structure are vital.

A task-oriented working technique will try to define what is necessary to fulfill the task and what is not. Applied to the workflow of the hydrogeological modeling approach, modeling systems and their connections and interactions are chosen according to the task in order to obtain a suitable result. Of course, this task will be managed according to the maxim "as much as needed and as few as possible". Simple modeling systems are preferred. Nevertheless, according to the modeling task, the connection of the simplest modeling systems can become very complex or the objective already needs a solution generated by a complex modeling system. This problem solving approach is called "top-down-programming" in computer sciences. The resulting workflow is a bit static.

A development-oriented research approach with an open task, as discussed by POPPER (1994) for the entire scientific history, tries to solve problems in the simplest way through falsification and elimination. Every time a solution is falsified – perhaps by a new problem definition – a better possible solution is researched. The proceedure results in a workflow that may be called iterative when it is converted to the modeling process and the interaction of modeling systems. The starting point is a simple modeling approach that involves only one simple modeling system. According to the requirements, other modeling systems are added. The workflow of modern techniques in computer sciences is quite similar: the "eXtreme Programming" (XP) technique is used for very efficient and customer-oriented program development. It is a very dynamic software development approach.

Both workflows have parallels to the hydrogeological modeling approach, and they are applied to the interaction of modeling systems. Thus, the contributions of HILL (2006) and GOMEZ-HERNANDES (2006) to the discussion of couplings of modeling systems are very helpful. Both scientists find different ways to model complex objectives and they emphasize the necessity of the application of interacting modeling structures for these complex tasks.

Of course, the tasks and research approaches are very diverse; the possible couplings of modeling systems are bound to the different aspects and must follow these objectives. For the couplings of hydrogeological modeling systems, as proposed here, the modeling systems for geology, infiltration water, the unsaturated zone, and numerical solutions for the saturated zone are considered with their relations in Figure 42.

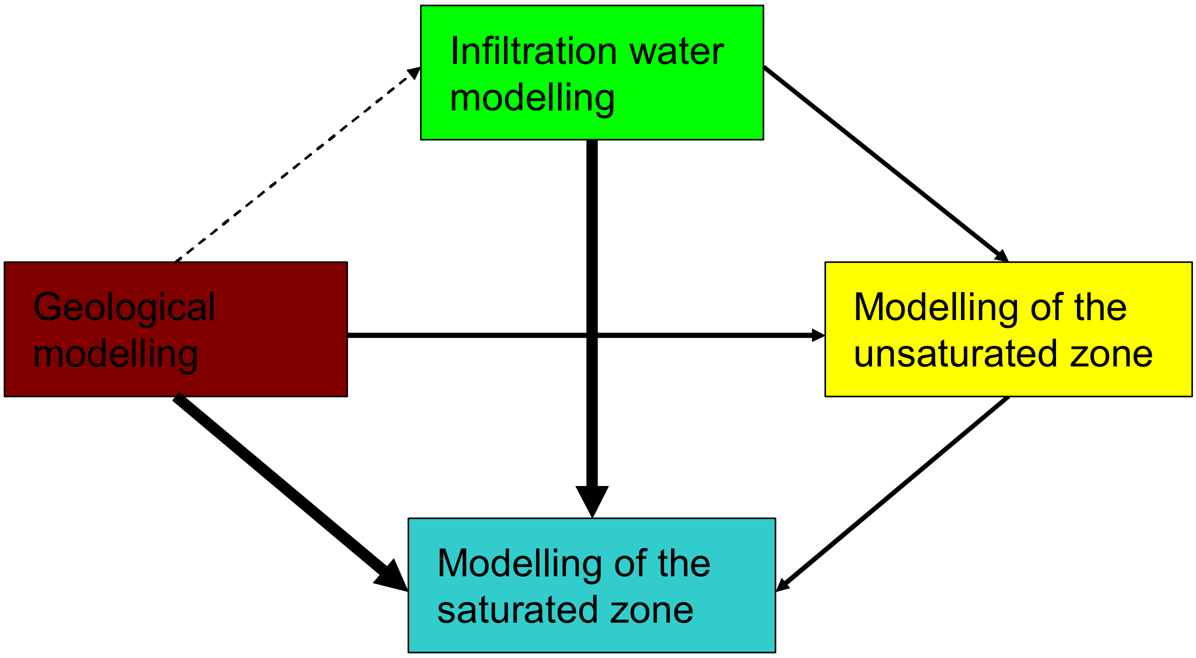


Figure 42: Overview of the considered modeling systems. The relations between the modeling systems can be configured in very different ways. This is shown in a schematic view.

These hydrogeological modeling systems have a definable border to the modeling systems of the atmosphere (climatic models), surface water, hydrochemistry, and land use, all of which will be mentioned occasionally. The systematic approach to the classification of interfaces for hydrogeological modeling systems can be transferred also to the interfaces of these adjacent modeling systems to a certain extent.

The connection of several modeling systems for the purpose of a complex hydrogeological modeling could be carried out in an ideal case, as with the object-oriented programming in computer sciences: each modeling system contributes to the division of tasks. The complete task can be made more transparent by looking at the connection of well-established and controllable modeling tools. Additionally, these tools are verified and proven.

The connection of modeling systems is not simple because the modeling systems take only distinct information – parameters or boundary conditions – from each other. Sometimes, a very intensive rework of one model as a "server" for the next modeling system is necessary. Considering the complexity of these tasks, it makes sense to consider the system of these interfaces theoretically and in the context of case studies.

As shown in chapter 2, static and dynamical modeling concepts should be differentiated in a fundamental way. The dynamical modeling systems for infiltration water modeling, unsaturated zone modeling and groundwater flow modeling depend on the conceptual model derived from the detailed geological model. This helps for setting up the model structure as well as for the generating the distribution of some parameters. A direct transfer is possible in rare cases. In general the geological structures must be classified in a new way, so that they fulfill the demands of numerical groundwater modeling.

To start with a systematic approach for diverse coupling possibilities, the first attempt focuses on the topics of modeling:

- HOLZBECHER ET AL. (2005) will define a model coupling as being “inter-compartmental“, if different compartments are modeled.
- The coupling will be defined as “intra-compartmental“, if the same compartment is considered in the modeling process.
- The connection of spatially or temporally different models based on the same modeling system is called horizontal coupling.
- The connection of models based on different modeling systems is called vertical coupling.

There is the possibility of an intra-compartmental coupling with a vertical structure. An example for this is the coupling of a groundwater flow model and a transport model in the saturated zone.

The composite systems described by HINRICHSEN & PRITCHARD (2005) distinguish four kinds of connections:

- A series connection occurs when the output of the first modeling system is connected to the input of the second modeling system
- A parallel connection will be obtained if both modeling systems get the same input and the composite system represents the sum of the individual outputs.
- The dynamic output feedback is based on a feedback interconnection, where the output of modeling system 1 is connected to the input of modeling system 2, and the output of modeling system 2 is connected to the input of modeling system 1.
- The static state and output feedback connection is used for a connection of a steady state model with a dynamic model of the same modeling system.

This classification is not used in this study, because this more mathematically oriented approach is not appropriate in the field of hydrogeological systems.

Another classification, described by MÖLDERS (2005), focuses on the data exchange:

- A “parameterization“ is defined as the direct setting of parameters and/or boundary conditions of a model based on a conceptual model. This is not a real coupling because the mathematical formulation of the model is lacking.
- A “one-way coupling“ is a connection from one modeling system to another. This form of coupling can also be referred to as sequential coupling.
- A system based on modeling systems that are connected in both directions may be called a “two-way coupling“, or a feedback coupled system. This type of coupling must be divided into two categories because the feedback can be either non-iterative (serially) or iterative (parallel). In a non-iterative feedback, the results of one modeling system are transferred to the next modeling system so that they are the input values for the next time step. For the iterative feedback approach, in the same time step, the iteration functions are repeated as long as a predefined minimum of the differences between iteration steps is not reached.

- Another possibility for data exchange that is not reported by MÖLDERS (2005) is the periodically synchronized coupling. In this type of coupling, the data exchange is reduced to discrete time steps. Thus, this is a special configuration of a non-iterative feedback coupling.

- If the modeling tools are connected so directly that they cannot be distinguished from each other, the coupling should be called “integrated coupling”.

The relation of two coupled modeling systems can be described in more detail by the terms weak and strong. The one-way couplings and the non-iterative couplings are weak couplings. Another criterion for the distinction is the number of transferred values (parameters and/or boundary conditions). Weak couplings can be characterized by the ratio of transfer parameters and by the total number of parameters. This ratio is low for weak couplings and high for strong couplings.

FÜRST (2004) classifies the model couplings that can be realized with a GIS into broad couplings and tight couplings. According to this classification, a tight coupling is characterized by an integrated graphical user interface (GUI). A broad coupling does not have this GUI, and thus the data exchange is realized via very simple data formats. This user oriented approach is not followed here. A graphical overview of the coupling possibilities is given in Figure 43.

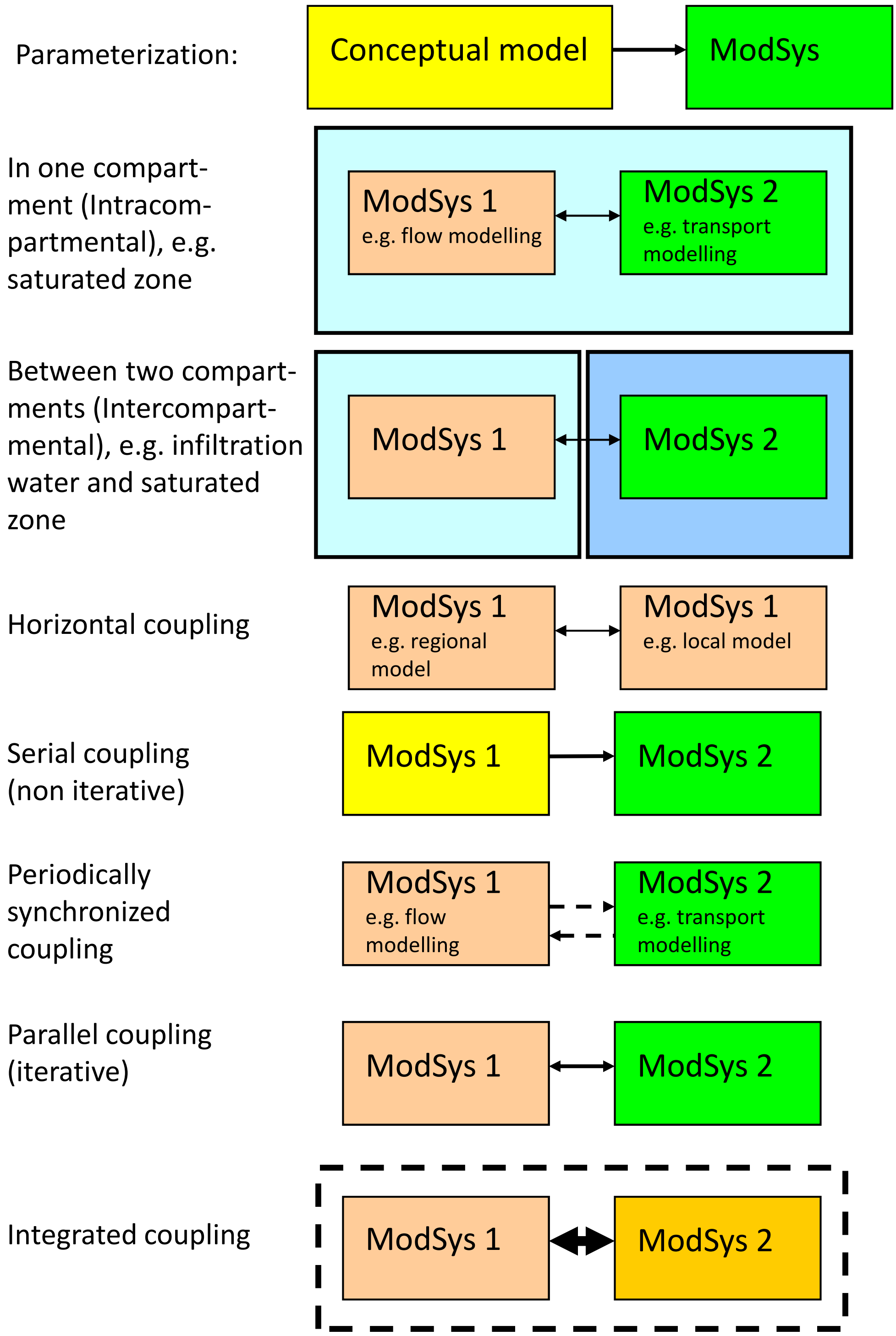


Figure 43: Graphical overview of possibilities for the coupling of modeling systems (ModSys).

The types of coupling – either classified according to modeling topics or the exchange focus – can be combined according to modeling tasks and available resources. Fundamental issues are the usage of couplings and the consequences for the application of the intended modeling systems.

The couplings and the questions of stability and dimensioning of coupled models will be extended in this chapter, according to Figure 44.

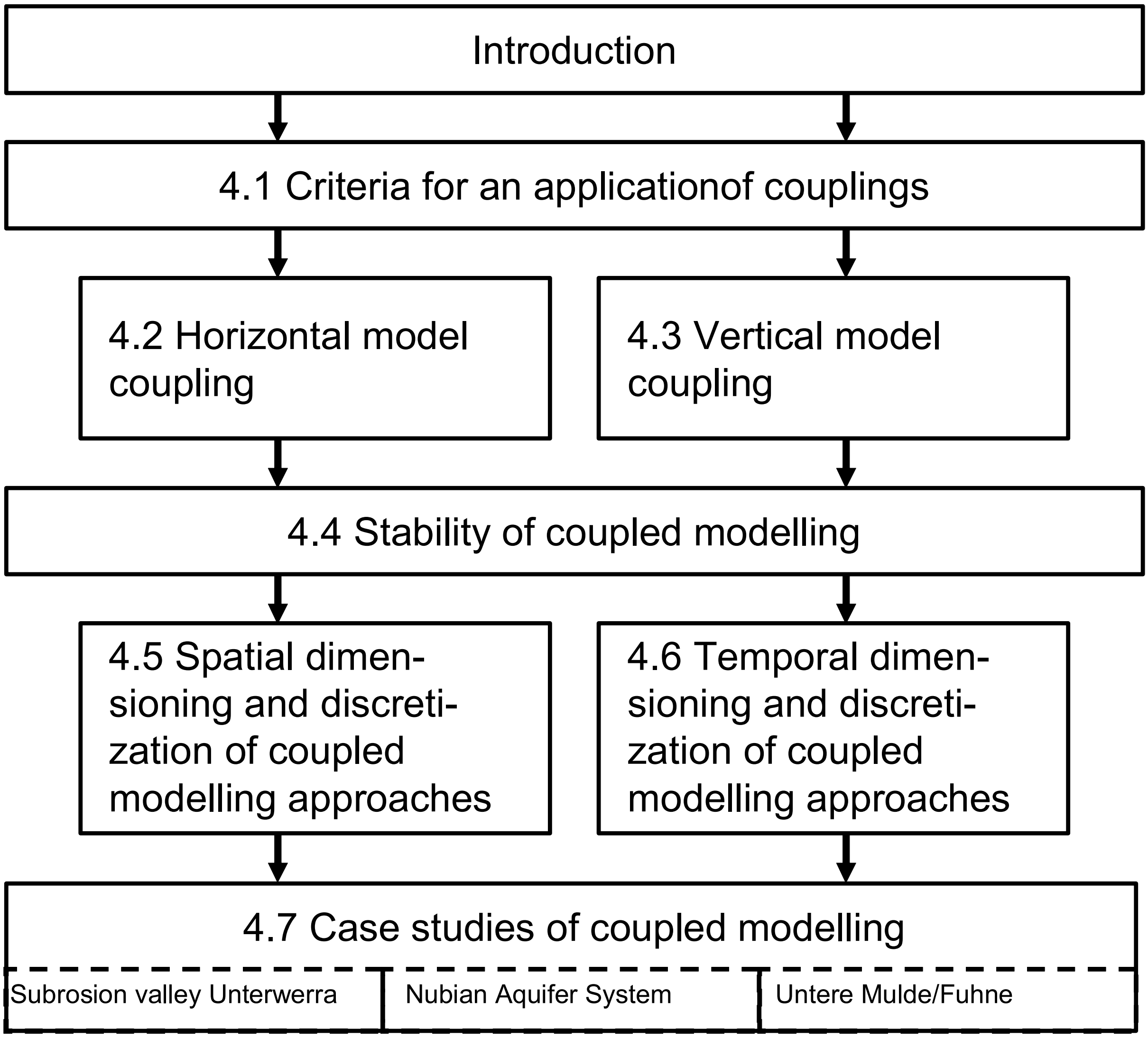
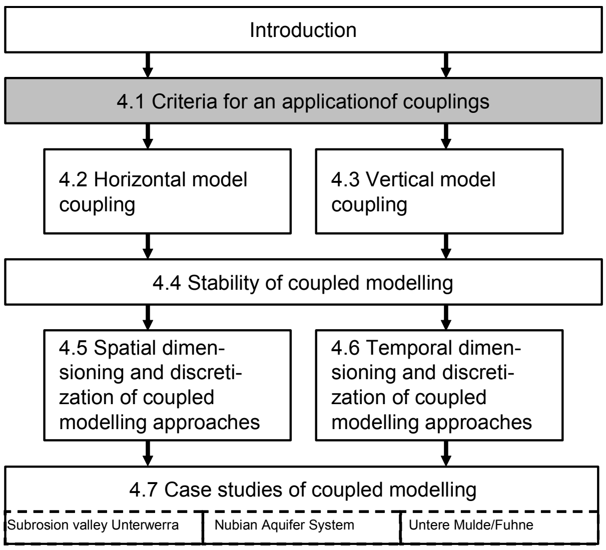


Figure 44: Graphical overview of chapter 4. For better orientation, this graphic will be shown as a miniature in the following subchapters.

4.1 Criteria for the application of couplings in hydrogeological modeling



Connections of modeling systems can be inserted at diverse points in the workflow according to the overall working procedures. A task-oriented workflow is obliged to set the insertion points very early according to predefined criteria. A development-oriented working approach will be confronted with the issue of inserting an additional interface several times during the workflow. In this case, the question of the suitability of an additional modeling system should be decided.

Besides the point of decision in the workflow, there are criteria for the decision as to whether a coupling of modeling systems is necessary at all. The systematic approach supports the decision of the type of coupling. Therefore, criteria for the choice of suitable modeling tools can also be derived from the necessity of a coupling. For all the applicable modeling tools it must be guaranteed that they fulfill the criteria that are set by the modeled processes according to the criteria in chapter 1.2.

At the beginning, the criteria for the application of a coupling are very general. A coupling is of course necessary if the objective criterion of the modeling cannot be adequately satisfied by an applied modeling approach. The determination of “adequately” is subject to many interpretations because normally this term will be related to the deviations from reality. This will be discussed later in this chapter. Another possible criterion may be the application and implementation of a conceptual model or the possibility of modeling a certain scenario.

The reason for the failure in reaching the objective criterion can be that certain parameters, boundary conditions, or initial conditions are not implemented in enough detail. However, there can be model-immanent reasons that lead to such a result, e.g. an insufficient resolution. Another reason can be – especially in the context of prognostic modeling – missing information that could be completed by the application of additional modeling systems.

Thus, values other than the criteria of the objectives can be used for the application of couplings of modeling systems, and these should be considered in detail as there are process values serving only as subordinate variables for the objective criteria.

Classical objective criteria in hydrogeological modeling are groundwater levels and water balances. These criteria can be important for the model result in their spatial distribution and their temporal dynamics. The couplings of this modeling approach must be considered under these aspects.

If only the spatial distribution or the temporal dynamics need to be improved by the application of an additional modeling system, a sequential coupling is in most cases suitable. This can be applied when only one of the modeling systems to be coupled fulfills this characteristic. If both, spatial and temporal dimensions need to be considered, a coupling with feedback must be implemented. This coupling via feedback may be iterative, periodically synchronized, or integrated.

Horizontal couplings of dynamical transient models should be calculated with feedback, either iterative or integrated, because these models are always spatially and temporally dimensioned. In addition, sequential couplings can be implemented for steady state models or static models.

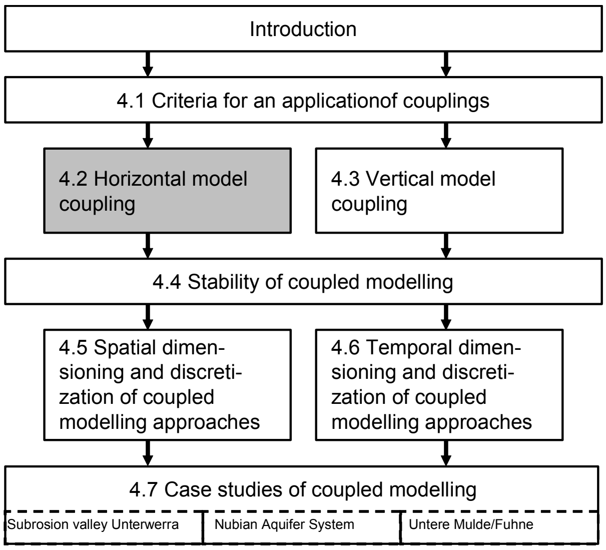
For all model couplings, the scales must be adapted to the coupling process. For purely spatial or temporal couplings (sequential couplings in most cases), this should be no problem. For the modeling systems that are connected by iterative couplings, this will lead to a disaggregation of the model calculations under the conditions of the highest resolution. In most cases, the resolution of the result is even higher than the necessary resolution and the resolution of each of the coupled models on account of the necessary iteration steps.

Iterative calculations generally require significant calculation time. In most cases, a parallel computing is not implemented for the modeling approaches. The periodically synchronized working approach has in thes cases some advantages.

For the coupling of modeling tools, GISs are often favored. Their applicability is readily recognized because they can be used to set spatial relations for the 2D datasets.

Furthermore, their data formats are widely supported, even by highly specialized modeling systems. Their deficiencies in the third spatial dimension and in the temporal dimension are most critical, especially for geologists. Whereas the missing third spatial dimension can be bridged by expert techniques and supported by some minimum features, dynamical couplings cannot be realized using a GIS. Consequently, in addition to the missing features and compatible formats of these standard tools, coupling of hydrogeological modeling systems involves significant effort with these techniques – beneath the issues of the objectives for a coupling which will be discussed in the next chapters. The only simplifying features are the modular structure of several modeling tools and the supply of defined and well-documented interfaces.

4.2 Horizontal model couplings



Horizontal couplings of models are suitable for modeling temporal or spatial sections in detail. In this case, the same modeling tool is used twice to connect a model with a high resolution (e.g. a local model) with a model of lower resolution (e.g. a regional model). The most important, but sometimes neglected, condition is the need for a higher resolution of the input data or for additional input data. Only in rare modeling approaches will the mere improvement of the discretization give a better result. This approach will not at all solve the issues of scale dependencies of parameters or boundary conditions.

In static models, a higher density of input data can be considered by inserting a horizontal model coupling. In dynamical modeling approaches, an improvement of the model can be achieved through a higher resolution of parameters or boundary conditions and a higher discretization.

In the next sections, the horizontal coupling of hydrogeological modeling systems will be considered in detail.

Couplings of geological modeling systems

The interfaces of two models should be considered for the geological modeling approaches that have been developed based either on the same (constructive or statistical) modeling methods or on different modeling methods. Examples for the first kind are couplings of models with a different resolution (something like a magnifier), and the second kind may be represented by an insert area with a high anthropogenic impact, such as an area in which open pit mining occurred. In both cases, there will be small differences at the edges of the two model areas; these can be resolved through adequate algorithms, as described i.e. in THOMSEN (2005), if the modeling systems are the same. If the applied methods are different, e.g. a mixture of statistical and constructive methods, a more pragmatic way, that will only adjust the results at the edges as described in HUBERT (2005), can be chosen. An image of clear “fractures” that shows the different concepts in detail is an alternative. For the latter approach, a general data concept must be created for a consistent result, as described in

THOMSEN (2005). For overlapping triangular meshes, this can be achieved through a combination of the two meshes with an increased resolution in these overlapping areas. However, this is only possible if both models were developed such that they were dependent on each other. In a normal case, the slices of the modeled bodies are not consistent, and this will result in very rough surfaces. This derives from the takeover of the differing net structures and reflects the lack of an adequate database of hard data in the overlapping regions. The pragmatic solution would be to completely cut off the data collectives in both nets in these overlapping regions. The representative parts would be extracted from both models that are connected and used as the database for a geostatistical interpolation. The point data sets of both models must afterwards be connected again. Additionally, the topological integrity of the bodies must be guaranteed, i.e., there must be no intersections of bodies and/or other slices for the models in this area. For models with a regular raster, there is a possibility of calculating averages in the overlapping regions. This will certainly result in additional fractures in these areas. For the application of constructive methods, the cleanest solution is the elimination and reconstruction of the intersecting areas.

Process-based or even dynamic geological modeling cannot be considered here because no investigations have been carried out in this field. A horizontal coupling would be very interesting, especially for these modeling systems, because this would enable modeling long time periods and large model areas.

Modeling of infiltration water and the unsaturated zone

In modeling systems for infiltration water and the unsaturated zone that involve soil water storage ("bucket models") (PFÜTZNER 1994, WESSOLEK 1989, HÖRMANN 2005) there is a possibility of inserting additional hydrological response units or of increasing the temporal resolution. A better result is achieved with a good resolution of input data without a horizontal coupling. For modeling systems working with empirical or statistical methods, this is not feasible. The possibility of a coupling would be desirable for modeling systems for the unsaturated zone that work with the Richards equation in three spatial dimensions, but as yet there are no approaches for any applications.

Numerical groundwater modeling systems

In MEHL ET AL. (2006), different methods of coupling for a modeling tool for the saturated zone are compared in regard to increasing the spatial resolution in an effective way. The concepts for such tasks are usually not very complex. These results and improvements for the spatial resolution can be transferred to the temporal dimension as well as in other cases where statistical methods in particular can be applied to spatial and temporal problems in similar ways.

The comparison shown in MEHL ET AL. (2006) of a locally densified discretization considers two kinds of coupling: sequential coupling and iterative feedback. Two models with a different discretization are created based on the same modeling system. The results of the model with the lower resolution are transferred to the model with the higher discretization. In the case of an iterative feedback, the models transfer their results as initial conditions and/or boundary conditions, and they calculate by iteration until both models reach the same values for the feedback parameters. Both models are predefined and are not changed during runtime. Such a concept can – aside from the described applications – also solve the problems of local (hydro) geological lenses and fading out layers.

The description of the feedback values plays an important role in horizontal modeling approaches. All kinds of boundary conditions can be used for the coupling because two identical modeling systems are connected only through different resolutions. For the described models, the objective criteria of the water levels and concentrations were taken, but the calculation values for transport of water (flow) or substances may also be used.

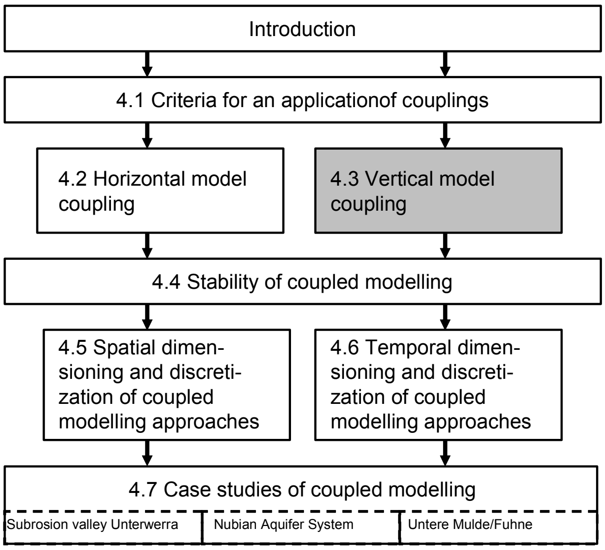
For some modeling tools, the horizontal coupling is integrated into the development process. This may be the capability of automatic time step control with the ability to predefine time steps for the output according to the necessities of the modeling task (and the user's requirements), or it may be the user-oriented improvement of the spatial resolution as described in (DIERSCH 1994, and DIERSCH 2005).

Hydrological modeling

In the context of climatic research, issues related to the effects of very sudden events are resolved through horizontal couplings of models. Detailed models with high temporal resolution are inserted into long-term models with a low temporal resolution, as described by VALDES (2005). Important time periods for these modeling approaches are the mid-term developments, such as the "small ice age" in the nineteenth century, the warm period in the Middle Ages, or short-term events, such as the sudden influence of freshwater into the North Atlantic Ocean that occurred 8200 years ago.

LEAVESLEY (2005) describes additional applications of horizontal model couplings that intersect with vertical but intra-compartmental model couplings. The model is a Global Climate Model (GCM) that must be downscaled such that it produces results for a higher temporal and spatial resolution. For this purpose, statistical methods (Statistical Downscaling, SDS) and methods of dynamical modeling via a Regional Climate Model (RCM) were applied to obtain better values for the monthly precipitation and temperature data from a climate station. Both downscaling methods evolved to be equally applicable, and a definite improvement of the dataset was achieved. The statistical method had the advantage of being dependent on a smaller amount of input data and thus was preferred. The aggregation of hydrological data for the parameterization of a GCM is not at all complicated, as described by MÖLDERS (2005). For this purpose, the values of the dominating classes, the mosaic approach, or arithmetical, harmonic, or geometrical averages are used.

4.3 Vertical model couplings



Vertical model couplings were developed and applied to the content-related extension of the models. For this purpose, in most cases, additional compartments of the water cycle or the transport of substances are integrated. The modeling systems that should be considered in hydrogeology in terms of model couplings are shown in Figure 45. The interfaces and strategies for a coupling of the highlighted modeling systems will be considered more specifically in the following sections.

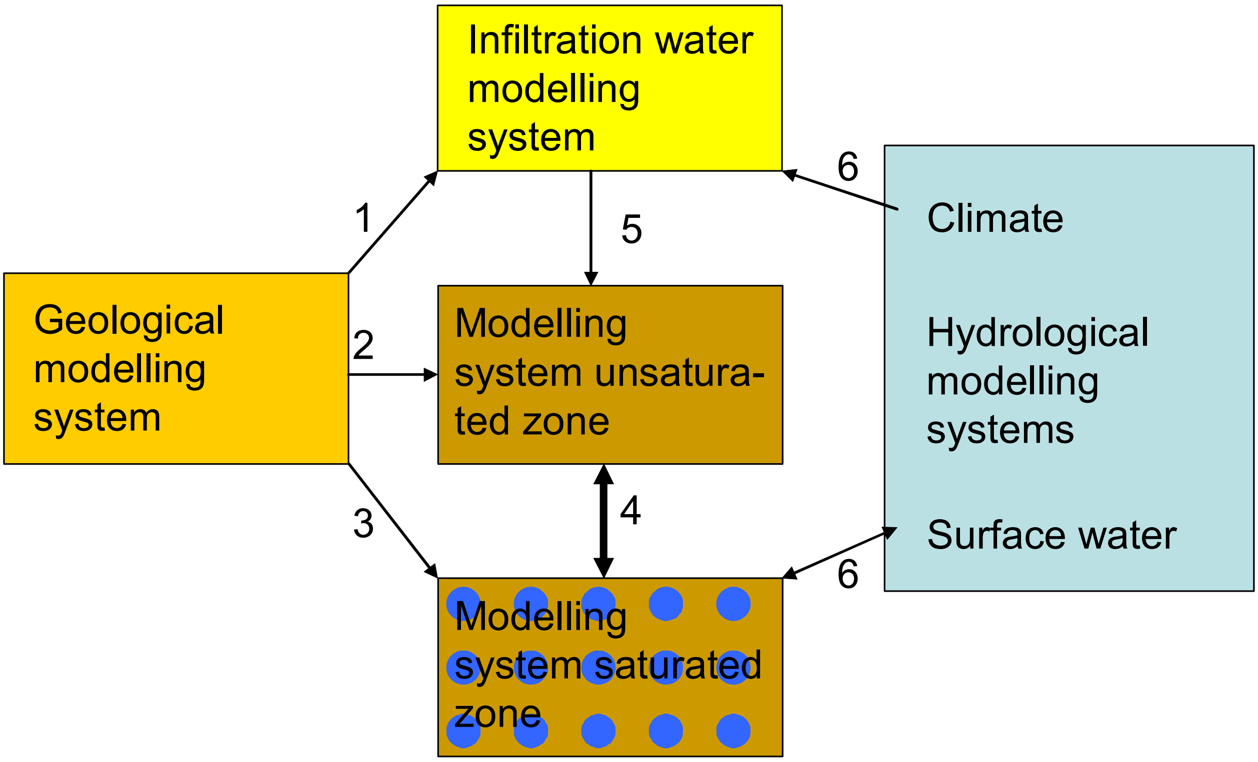


Figure 45: Modeling systems with vertical coupling that should be considered in hydrogeological systems. The arrows indicate the direction of the coupling. The numbers refer to the sections in the text that contain the corresponding explanations.

According to the numerous connections in the graphics, the importance of a modeling system can be estimated. Nevertheless, only a more detailed view of the interfaces will indicate the real efforts that is required for a good coupling. Three modeling systems are in the centre of the considered model couplings: the geological modeling system, the modeling system for the unsaturated zone, and the system for the saturated zone. The numbers and types of the vertical couplings were distributed irregularly.

The numbers in Figure 45 show the text structure for the description of the interfaces.

1: Interface geological modeling system – infiltration water modeling

The geological model can be used to transfer the parameter values for the soil substrates to the modeling system for infiltration water. The description according to the systematic units for soils (soil classes, types, and subtypes) is in most cases not very helpful because the empirical or soil storage modeling systems depend on specific parameters that can only be derived from soil substrates. These parameters are field capacity, wielding point, and hydraulic conductivity. Additionally, many soil maps are only made to estimate the value of agricultural soils and do not cover soils in forests. This is why they were not investigated. The forestal soil maps show only soil types and no substrates. Geological maps, which are important databases for geological modeling, can also be used to derive the needed substrate information for the infiltration water modeling – on farmland as well as in forests. A high-resolution geological model will also feed these data in an adequate way. With respect to the stratigraphical orientation of geological modeling systems, an additional interpretation is often needed. A lithologically oriented model, in comparison to a stratigraphical model would make it much easier to interpret the desired values, and it could directly provide for the parameter distribution via a model coupling.

Feedback is not implemented because the geological modeling system is not able to take any information from soil maps or from the parameter distribution of the infiltration water modeling system. Therefore, the coupling must be classified as a sequential coupling. For the case of a transfer of a conceptual geological model, the coupling is reduced to an ordinary parameterisation.

Transport modeling systems for the unsaturated zone need additional parameters that cannot be derived directly from a geological model.

2: Interface geological modeling systems – modeling systems for the unsaturated zone

Modeling systems for the unsaturated zone can obtain diverse parameters from the geological model. In compliance with the first interface, this interface also represents an application of sequential coupling. A pure parameterization is not suitable for a differentiated modeling approach. The vertical structure of the unsaturated zone is the most important factor in this modeling task. Further, for a modeling approach for a soil water storage (“bucket”) model, the parameters of the porosity or the field capacity are needed for each layer. For modeling systems that are based on the Richards equation, the minimum factor is the determination of the parameters porosity and hydraulic conductivity. Additionally, the initial conditions of the model for the unsaturated zone play an important role. These values cannot be derived from the geological model in any way. They must be set to a useful value. From this list of parameters, it is obvious that a direct transfer of data from a stratigraphically oriented geological model is also not possible. At the least, a lithological interpretation and subsequent assessment of the lithology according to the parameters mentioned above is necessary. This problem will be addressed again in the description of the interface between geological modeling systems and groundwater modeling systems for the saturated zone.

For a three-dimensional model of the unsaturated zone, the additional problem arises for layers, but this problem does not cover the entire model area. This problem is discussed in another chapter in more detail because the numerical solvers involved for the unsaturated zone are also used for the saturated zone

Transport modeling systems for the unsaturated zone are additionally dependent on a parameterization from the geological model in terms of sorption parameters and degradation parameters. This is not possible in most cases based on a pure geological model. For this task, the contents of clay and humic substances are necessary. They can be derived from geological models, but only with extreme interpretation effort. Several additional parameters for the transport model have nothing to do with geological structures and derived parameters. Thus, a coupling of a geological model with a transport model must be defined as a weak coupling.

3: Interface geological modeling systems – modeling systems for the saturated zone

The transfer parameters of this interface cannot be derived directly from the geological model. For three-dimensional numerical groundwater modeling, the structures and the hydraulic conductivity and porosity are the first parameters that can be taken from the geological model. This coupling must be considered as a strong connection because most of the input parameters, including the most important ones, are set in this way. It is a sequential coupling because normally there is no feedback. An exception could be subsidence areas affected by groundwater extraction where the geology is also affected to a minor extent.

A very important issue is the distinction between the saturated and unsaturated zone. This differentiation is not relevant for a geological model and thus is not subject to the modeling process. The modeling systems for the saturated zone, according to the definition, have their top at the groundwater surface. This is why the geological models must be cut off at this horizon. A second difficulty in the generation of a structural model for numerical groundwater modeling arises from the numerical constraints: all layers must exist in the entire model area – i.e., there is no possibility for a direct transfer of fading out layers and geological lenses. In most cases, larger faults also cause problems for the structural model. Additionally, a minimum thickness must be guaranteed for each layer owing to numerical demands. Especially in areas with a high anthropogenic impact, such as open pit mining areas, very steep angles at the edges of the pits must be converted to adequate and numerically stable model structures. The averaging between the layers for certain parameters was explained in chapter 3.4.2, and it must be taken into consideration for the creation of a structural model. GISs can be very helpful for the described reworking of the model.

When the geological model is built on a stratigraphical classification, the conversion can be very complex, with a nearly complete revision. A lithological model has to be generated in the first attempt. The stratigraphical classifications, which are vital for the generation of a consistent geological model, are not interesting for all of the considered vertical couplings. They cannot be transferred directly to hydraulic conductivities and porosities. The lithological information can serve for the derivation of these parameters, and afterwards, a spatial distribution can be created through an adequate interpolation technique. An indexing system has been established as a suitable step, especially in the context of a calibration that must be carried out later. ANDERMAN & HILL (2000) propose a tool that helps to convert geological model layers to layers of a numerical groundwater model. This tool does not consider or solve the problems with the unsaturated zone.

Transport models of the saturated zone require several additional parameters including the sorption coefficient. These parameters cannot be derived from the geological model, as already described in reference to the unsaturated zone. One possibility is using the clay content or the content of humic substances. For the parameter dispersivity, not only the geological model with some vague information about heterogeneities of the rocks but also the overall geometry of the entire model area should be considered (KINZELBACH 1987). HAEFNER & BOY (2003) describe a coupling technique for the modeling systems for flow and transport in the saturated zone that modifies the spatial resolution according to the concentration of substances in the transport model.

4: Interfaces of the modeling systems for the unsaturated and saturated zone

This interface can be implemented as a parameterization or as a sequential, periodically synchronized, iterative, or integrated coupling. For many modeling tasks, a direct transfer of the infiltration rate as a parameter or boundary condition for a numerical groundwater model is sufficient. In these cases, an interface between the unsaturated and saturated zone models need not be considered. In areas with large depths to groundwater and/or impermeable layers in the unsaturated zone, these conditions should be recognized through a detailed modeling. This is especially important in cases of dynamical analyses performed by the model.

The feedback value from the saturated to the unsaturated zone model is the groundwater level. If the zone of the groundwater level fluctuation is small, e.g. in the case of layers with a low hydraulic conductivity, the feedback can be neglected. In these cases, a sequential model coupling is a suitable interface. An integrated coupling should be used only in rare modeling approaches because these model couplings are comparably unstable and, therefore, very computationally intensive. The reason for this behavior is the drying of the layers in longer drought periods. This causes, according to the Richards equation, the reduction of hydraulic conductivities, and consequently a further infiltration is prevented (see chapter 3.3.2). Furthermore a very high horizontal and vertical discretization of the unsaturated zone is necessary.

The few transfer parameters or boundary conditions for the non-integrated solutions indicate that the coupling is quite weak. In practice, a periodically synchronized coupling should be preferred. For an integrated solution, several parameters could be used by both modeling systems, but this must be decided according to the modeling approach. This dual use of parameters strengthens the coupling. Sequential and integrated solutions are implemented in several modeling systems (NISWONGER ET AL. 2006, DIERSCH 2005).

5: Interface of the modeling systems for infiltration water and the unsaturated zone

The transfer between infiltration water modeling systems and modeling systems for the unsaturated zone is rarely used. This is reasonable because the thickness of the unsaturated zone is small and thus can be neglected. Another possibility could be the insertion of a soil water storage (“bucket”) modeling system that can integrate the unsaturated zone. A third possibility would be the integration of soil water budget modeling into a modeling system that works on the basis of the Richards equation for the unsaturated zone. This solution is almost never implemented because parameterization is so complex. Feedback for this interface is not necessary. The only reason for adopting such a modeling approach is parallel feedback of the groundwater table.

The transferred parameters and/or boundary conditions are runoff values. Therefore, this also is only a weak coupling.

6: Interface between modeling systems for hydrogeology and hydrology

These interfaces are not considered here in detail, but a few characteristics should be discussed. The interfaces between the modeling systems for groundwater and surface water can be implemented in a couple of ways. In both systems, water budgets and water levels are considered in connection to each other. From the point of view of a groundwater model, the surface water is implemented either in a Dirichlet or in a von Neumann boundary condition. For very small creeks or grabens, which can become dry during the modeling time, the implementation of constraints makes sense because it ensures that these weak surface water bodies will not infiltrate or exfiltrate at certain water levels. The transfer of the water levels in the surface water is important for the determination of the boundary conditions of the groundwater model. The groundwater flow model calculates the water exchange internally on this basis. The water level of the groundwater is not relevant to the surface water. For this modeling system, the water budgets of the exchange must be taken into consideration (FRÖHLICH ET AL. 1998). These differences in the determination of a feedback-coupled model should be respected. This interface can be regarded as a weak coupling of modeling systems. The couplings can be implemented as sequential couplings, periodically synchronized couplings, iterative couplings or – in rare cases – even integrated couplings. The temporal discretization and, to the same degree, the coordination of the time steps is of high importance because both systems behave completely differently in this dimension. For the iterative and integrated couplings, this can lead to a very high computing time. The spatial discretization can also be problematic because the water exchange via the bottom of the surface water body must be calculated. If the surface water is defined as an internal boundary condition, the elements in the groundwater model must be very small and narrow. Especially for finite difference methods, the models without a horizontal coupling will include many additional elements. A horizontal coupling will perhaps cause additional problems. Add-ons or additional modules for the modeling tools normally support this task and supply additional adequate coupling methods.

Couplings to the mainly statistical rainfall-runoff modeling systems and to the numerous soil-vegetation-atmosphere transfer schemes (SVATS) are not considered here. They are very diverse in their structure, and thus a coupling could connect to various interfaces.

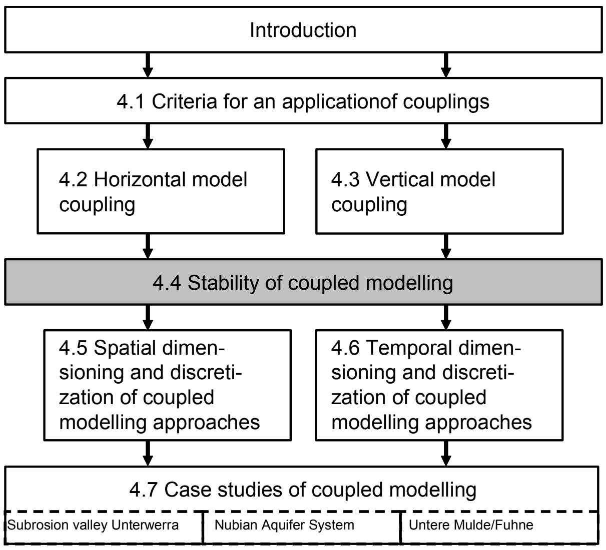
The interface between climatic models, weather models, infiltration water models and soil water storage models becomes increasingly important in the research on the effects of climatic change. Increased computational power now allows for the consideration of soil water contents and of complete soil water balances. This was neither necessary nor possible for the global climate models (GCM) in the past. Aside from this research topic, this interface can be defined almost always as a parameterization or a sequential coupling. Transfer parameters from the atmosphere to the infiltration water model or the soil water budget model are the precipitation and the potential evapotranspiration, which are calculated according to the methods described in chapter 3.2.1. For the coupling of GCM and infiltration water modeling systems, the scaling problem must be taken into consideration because the differences in the scales are very large. This problem can be solved through adequate statistical methods (statistical downscaling, LEAVESLEY 2005) or methods that are closer to reality (dynamical downscaling, LEAVESLEY 2005). These latter dynamical methods have the disadvantage of being very computationally intensive. This results not only from higher spatial resolution but also from higher temporal discretization.

The coupling of hydrological and hydrogeological modeling systems introduces the question of different spatial and temporal scales. For the interfaces of hydrogeological models only, this topic is normally of minor importance. Parameter distributions should be adapted to these differences; otherwise the stability of the models decreases rapidly, especially for iterative or integrated couplings. Some solutions – such as the coupling of the temporally and spatially very high discretized soil water budget models and groundwater models with GCM – cannot be implemented at all at present owing to technical problems. Their local to regional scale or mesoscale areas are not compatibla with the global scale of the GCM (BLÖSCHL 1996).

Couplings of modeling systems in environmental geology

Modeling systems in environmental geology have in most cases interfaces that are similar to the already mentioned couplings. The primary difference is the focus on transport simulation. Another particular feature is the vertical coupling of two static modeling systems, as in the case of a three-dimensional distribution of contaminants based on a geological model. A pure interpolation will be nearly impossible on account of the parameterization according to the substances and the advective component of the transporting medium. The only possible solution for this case is coupling with a dynamical model. In practice, it is often necessary to make compromises that adapt the parameters for geostatistical interpolations to the geological information.

4.4 Stability of coupled modeling approaches



In the previous chapter, the unstable behaviour of coupled modeling approaches was mentioned several times. It will now be briefly considered in a systematic way.

4.4.1 Stability of modeling systems

Most modeling systems are non-linear, i.e., a change in a certain variable (initial condition, boundary condition or parameter) will not produce a proportional change in the modeling result. Each modeling system has its own instability phenomenon, as HINRICHSEN & PRITCHARD (2005) point out for numerical solutions of differential equations with diverse (mostly multi-step) methods. In some cases, the solution diverges rapidly, and in other cases it oscillates as a result of very small rounding errors.

The examples given by HINRICHSEN & PRITCHARD (2005) are bound to time-dependent models, but the question arises, as to whether there is something like a “spatial instability”. This must be distinguished in detail from spatial heterogeneity. Spatial instability generally occurs in cases of extrapolation. Some interpolation methods, e.g. most geometrical methods, avoid this phenomenon, but some others, e.g. the geostatistical methods, are very sensitive to extrapolation. Robust methods can also become weak if the GRID dimensions and some calculation parameters (e.g. the number of regarded neighbours or the search radius) are poorly defined.

All these considerations lead to the following classification of instabilities of the modeling systems and of their numerical solvers.

1. Numerical solvers of differential equations:

Many modeling systems are based on the solution of differential equations. One reason for instabilities may be related to the numerical solvers. In dynamical modeling systems, the interpolation methods for the time step length dominate the weakness or robustness of a model. Time interpolative methods, such as the Runge-Kutta or the Adams-Bashforth method, may enhance the performance and avoid early instabilities, but with a poorly defined time step length, they will also produce divergent or oscillating models.

2. Formulation of differential equations:

In some modeling systems, the formulation of the differential equations or matrix operations is poorly defined. These modeling systems are normally disqualified in the verification step of the modeling system.

3. Model resolutions:

The dimensioning and resolution of a model may be poorly defined. In the time domain, one possible reason for instabilities is that time steps are set too long. In the spatial dimension, the interpolations are the main reasons for instabilities, as described above. Dimensioning and model resolutions must be compatible with each other.

4. Input data:

Input data are a significant source of model instabilities. In the spatial dimensions, the thredimensional models are often good examples. For the vertical dimension, the database is often so sparse that either the resolution of the result must be set very low or the interpolation algorithm is required to cover the gaps in the database. In transient models, the initial conditions must be chosen very carefully – on the one hand, to avoid a long phase of adapting to real conditions, and on the other hand to avoid divergent models.

4.4.2 Stability of couplings

Regarding the estimation of the instabilities of couplings of modeling systems, a new level must be considered.

At first glance, the coupling of modeling systems should lead to a sum of the results. A more careful consideration indicates that the high non-linearity of hydrogeological modeling systems does not support this expectation. The estimation of instability is not merely a sum of the tendencies to instability of the joined modeling systems.

The hope of stabilizing a weak model by coupling another modeling system to substitute for the weak, and in most cases sensitive, parameter or boundary condition is not realistic. The time-dependent or spatially distributed function will generate more instability owing to the greater diversity of input values.

For the coupling methods, a few rules of thumb can be outlined.

Parameterizations and sequential model couplings normally should result in stable joined models if both connected models are stable. Instability of the independent model can easily be identified, filtered, and corrected before the parameterization of the dependent model.

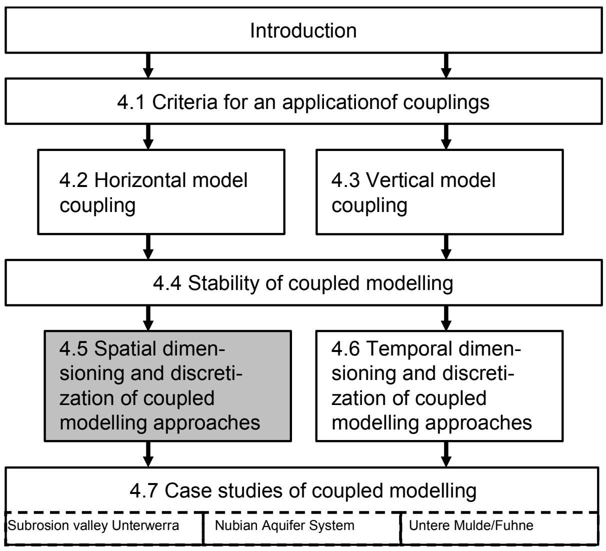
Periodically synchronized model couplings are vulnerable to unstable behavior only if the number of transfer parameters is high and the scales of the models are significantly different. In these cases, even the coupling of two stable models can be unstable. The application of so-called effective parameters may be one reason for this result. These effective parameters are described in BEVEN & KIRKBY (1979) and WANG ET AL. (2006). If the resolution of this parameterization does not fit the resolution of the necessary parameterization of the other connected modeling system, the entire coupling becomes unstable. Typical examples for this case are couplings of GCMs and soil water storage modeling systems or groundwater modeling systems.

The behavior of non-iterative couplings is similar to that of periodically synchronized couplings.

The most serious problems arise for iterative couplings and integrated couplings. Here, small changes in the spatial and/or temporal discretization dominate the status of the calculation steps. Whereas this problem is solved in the integrated modeling systems and modeling tools during the processing of the models, the iteratively coupled modeling systems internally work independently of each other. In this case, the transfer of data is bound to the skills of the scientists in programming the interface and to their knowledge of the sensitivity of these modeling systems to the transferred parameters. On the other hand, there are additional possibilities for the modeler to control and correct the values, e.g. in the case of numerical errors.

Finally, it must be stated that for all couplings – even in the case of the already well-established coupling of groundwater flow and transport modeling systems – the modeler must intervene in unusual or awkward conditions, perhaps via programming. Predefined programming interfaces support these approaches to a limited degree but they also restrict further developments.

4.5 Spatial dimensioning and discretization of coupled modeling approaches



The spatial dimensioning of coupled modeling approaches should be oriented completely differently from the dimensioning of the standalone modeling systems. Even the scale definitions of the connected modeling systems may differ widely.

KOLTERMANN & GORELICK (1996) connect the definitions of their scales directly to the geological dimensions: sedimentary basins (10^5 m), depositional environments (10^3 m), channels (10^2 m), stratigraphic features (1 m), flow regime features (10^{-2} m), and pores (10^{-3} m). VAN DE GIESEN ET AL. (2001) define the terms of scales and dimensions more widely. The scale of a process is defined according to its characteristic area. This connects the question of the dimension to the considered process. Non-linear behavior and variability depend largely on the considered hydrological processes. On the other hand, these processes are connected to certain scales. Thus, processes are directly connected to the range of model results. The process scale and the scale transition are fluent for some hydrological processes, in spatial as well as in temporal dimensions. For other processes, such as precipitation, there are obvious discontinuities observed in a scale transition (BLÖSCHL 1996). VAN DE GIESEN ET AL. (2001) connect the continuity of the scaling directly with the dimension of the model that is defined by the number of parameters or variables. As an example of a rather discontinuous scaling, the actual evapotranspiration is demonstrated.

In general, the very controversial discussion about scaling should be classified, according to BLÖSCHL (1996), into a process, measuring, and modeling scale. The process level in geological models is very difficult to determine. Therefore, only the dimensions of the results of these processes can be taken into consideration, as suggested by KOLTERMANN & GORELICK (1996). Thus, these scales also have a minor influence on the models that are created based on couplings with geological modeling systems.

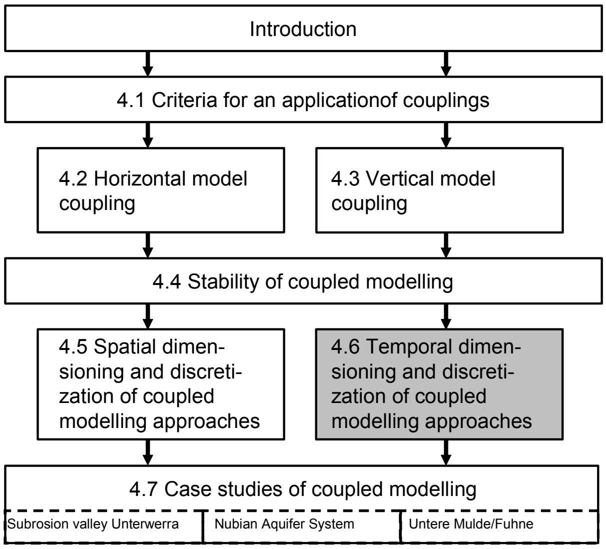
A good way to demonstrate the dimensioning, as well as the problems thereof, is given in regards to the modeling systems for geology, the saturated zone and the unsaturated zone (see Figure 45).

In the setup of a geological model, no boundary conditions are preset. This undefiniteness is independent from the application of statistical or constructive modeling methods. The dimensioning of the model area, therefore, is open to the limitations of the modeling objective. The discretization must be bound directly to the smallest units that need to be modeled. Similar conditions are obtained for the development of a model of the unsaturated zone. According to the mainly vertical structure, the dimensioning of this dynamical model is rather simple. The discretization is limited, to a minor extent, because the parameters cannot be disaggregated without limits. In the vertical direction, the discretization must be very high to fulfill the conditions of some modeling systems. However, this has no influence on the model coupling or on the coupled models. For the groundwater flow model, the dimensioning is bound to the boundary conditions. Here, the process scale limits the model dimensioning. Stable and strong boundary conditions are rarely found on a local scale. Therefore, the dominating dimension of groundwater models is found on the regional scale. On the other hand, the spatial discretization is limited by numerical rules to a minimum resolution, but the maximum resolution is set only by technical limits; thus, in this situation the modeling objectives clearly dominate the model layout. For the vertical discretization, see chapter 4.3. A criterion for the spatial discretization can also be obtained from the representative elementary volume (REV) if the resolution is so high that porosity and hydraulic conductivity cannot be regarded as a continuum. In this case, other systems, such as more adequate modeling systems, must be chosen. Defining something similar for infiltration water, soil water storage, or precipitation-runoff modeling systems (a "Representative Elementary Area" or REA) is impossible according to BLÖSCHL (1996) on account of the high heterogeneity of various necessary parameters.

There are other reasons why the discretization should not be too high. Most of the parameters of the considered models are not supported by field investigations in an adequate range. In most cases, there is also a large difference between the (geostatistically determined) range of parameters and their sampled range. By employing adequate interpolation methods, a parameter distribution can be calculated. If the sampling is not adequate, the result will be considered quite weak and uncertain.

For couplings with numerical runoff models or models of the atmosphere, the boundary conditions of these modeling systems dominate the dimensions of the coupled model.

4.6 Temporal dimensioning and discretization of coupled modeling approaches



Just as for the spatial dimensioning, the temporal dimensioning and discretization must follow different rules when modeling systems are coupled.

The temporal scales are characterized by time steps of several minutes, from very short-term storm events to geological processes of several millions of years. If the geological processes are not considered, the upper limit normally is a time frame of 100 to 200 years, or perhaps even less. Modeling approaches, such as those of CLAUSSEN (2005) or GOSSEL ET AL. (2004) are somewhat rare.

For coupled models, the model dimensions and discretizations of the connected models should be considered first. In the simplest case, the dimension of the longest model process can serve for the dimensioning of the maximum model period/timestep. The highest discretization of one of the coupled models can be transferred to the other model(s) as well.

The types of coupling have a significant influence on temporal dimensioning.

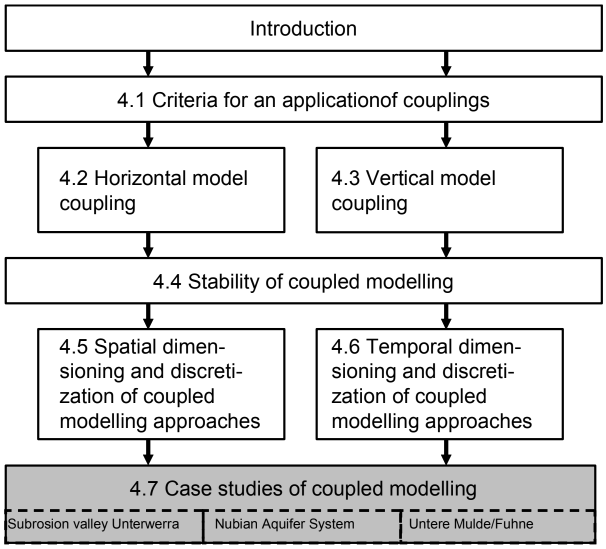
In sequential coupling, the modeling systems do not need to be synchronized. In the first modeling system, all values that need to be transferred to the other modeling system, such as parameters or boundary conditions, can be calculated. This calculation is thus completely independent from the other model. In couplings with a static modeling system, e.g., a geological modeling system or a steady state groundwater model, the temporal dimension can be neglected completely.

In a periodically synchronized coupling, but only in certain predefined time steps, a coupling is inserted. In this case, the coupled modeling systems can, to a certain extent, work independently of each other. This is especially interesting for internal iterations of the modeling systems because the models can run parallel to each other.

Only the iterative and the integrated coupling depend on the complete timing of both modeling systems. In the simplest case, this results in an adaptation of the time steps of the model with the highest discretization to the other model for the entire model time. In an awkward case, the discretizations are very heterogeneous and cannot be synchronized. In such cases, the time steps become very short. In these approaches of model coupling, the interface should be controlled by a regulating value so that the most obvious discontinuities can be avoided through a reduction of the time step length. In most cases, integrated systems with an automatic time step control (e.g.

DIERSCH 2005) have this function. In the case of unstable models or model couplings, the computing times can become very long owing to these control functions.

4.7 Case studies for coupled modeling approaches



Some examples from the literature demonstrate the use of couplings of modeling systems.

KUBATZKI & CLAUSSEN (1998), CLAUSSEN & GAYLER (1997), and CLAUSSEN (2005) describe the coupling of a modeling system for climate change with a modeling system for ecosystems in the desert area of Northern Africa – not for the recent climatic changes but for the Middle Holocene. In this coupling, the climatic model receives initial values for the parameters and boundary conditions. This is used for a first scenario, which is transferred to the modeling system for ecosystems. This modeling system returns corrected input parameters for the climate model for the same time step. Of course, the modeling system for the ecosystem needs additional parameters and boundary conditions, but these are not changed during the iteration steps of the time step. The results of the modeling system for the ecosystem can be used (after the iteration) as input parameters for the next time step (one year, constant time steps). According to the investigations, it takes six years to eliminate all of the trends that result from the initial conditions of the scenario. This coupling procedure was named “asynchronous modeling“ by CLAUSSEN & GAYLER (1997). This modeling procedure is, in the end, a transient modeling approach with an iterative step at the beginning, where the results are taken (owing to certain criteria, in this case the missing trend) as a steady state result. In the systematic view presented above, the coupling is (after the first iteration steps) a vertical, inter-compartmental, periodically synchronized model coupling.

A typical modeling task of numerical groundwater modeling is the calculation of the spreading of hazardous substances in the groundwater. The sources of the hazardous substances are hazardous waste dumps, accidents, etc. GOSSEL ET AL. (1998) describe the application of such a coupling for an investigation area in the northern part of the Federal State of Lower Saxony, near Hamburg. This coupling of groundwater flow and transport should be classified as a vertical, intra-compartmental, integrated model coupling. In several modeling approaches of this type, the flow model is regarded (and calculated) as steady state and the transport is calculated as transient, whereas in other case studies both are calculated as transient.

Very often, the numerical groundwater flow models are coupled to surface water models (e.g., HOLZBECHER 2005) or groundwater recharge models (e.g., PFÜTZNER 1994). The vertical and inter-compartmental couplings can vary widely, ranging from pure parameterizations to integrated model couplings. Additional case studies are presented in the next chapters to complete also these approaches.

The creation and transfer of differentiated geological models for the numerical groundwater modeling is rarely described in detail. SOMMER-VON JARMERSTED (1992) uses fairly rough structures that are as yet not completely modelled in three dimensions. In the descriptions of SCHAFMEISTER-SPIERLING (1990) and SCHAFMEISTER (1998), principle case studies are the focus. All examples are vertical, inter-compartmental, sequential (one-way) couplings. In the following chapters, these types of couplings are presented in detail.

4.7.1 Subrosion valley Unterwerra

For the complete model of the subrosion valley Unterwerra several coupling approaches were developed.

The geological model that was generated with constructive methods was transferred to a hydrogeological structural model. This solution was extremely labor-intensive because the conditions of the numerical groundwater model accept only layers that exist in the entire model area. Thus, not only the structures but also the parameterization had to be completely reestablished. Sequential coupling via the model structures offers many solutions, such as those described for the automatic conversion in ANDERMAN & HILL (2000). Conditions such as the minimum thickness and the fading out Quaternary layers at the edge of the valley, as well as the Quaternary sediment fans in the area of the hard rock aquifer, lead to problems that are difficult to solve. The horizontal coupling of the soft rock aquifer (valley aquifer, Quaternary) with the hard rock aquifer (sandstone aquifer, Lower Trias) is quite stable.

The parameterization of the numerical groundwater model was based on the results of the analytical calculation from the field investigations. A pure coupling of the results with the geological model would not have been reasonable and could not be used for further predictive results. Such a pure coupling would be possible in the numerical groundwater modeling approach.

The infiltration water model that was calculated according to the method of WESSOLEK ET AL. (2004) and the results were sequentially coupled to the numerical groundwater model. This coupling approach also turned out to be quite stable.

The coupling approaches of the central models for the geology, groundwater recharge/infiltration water, and groundwater flow are shown in Figure 46.

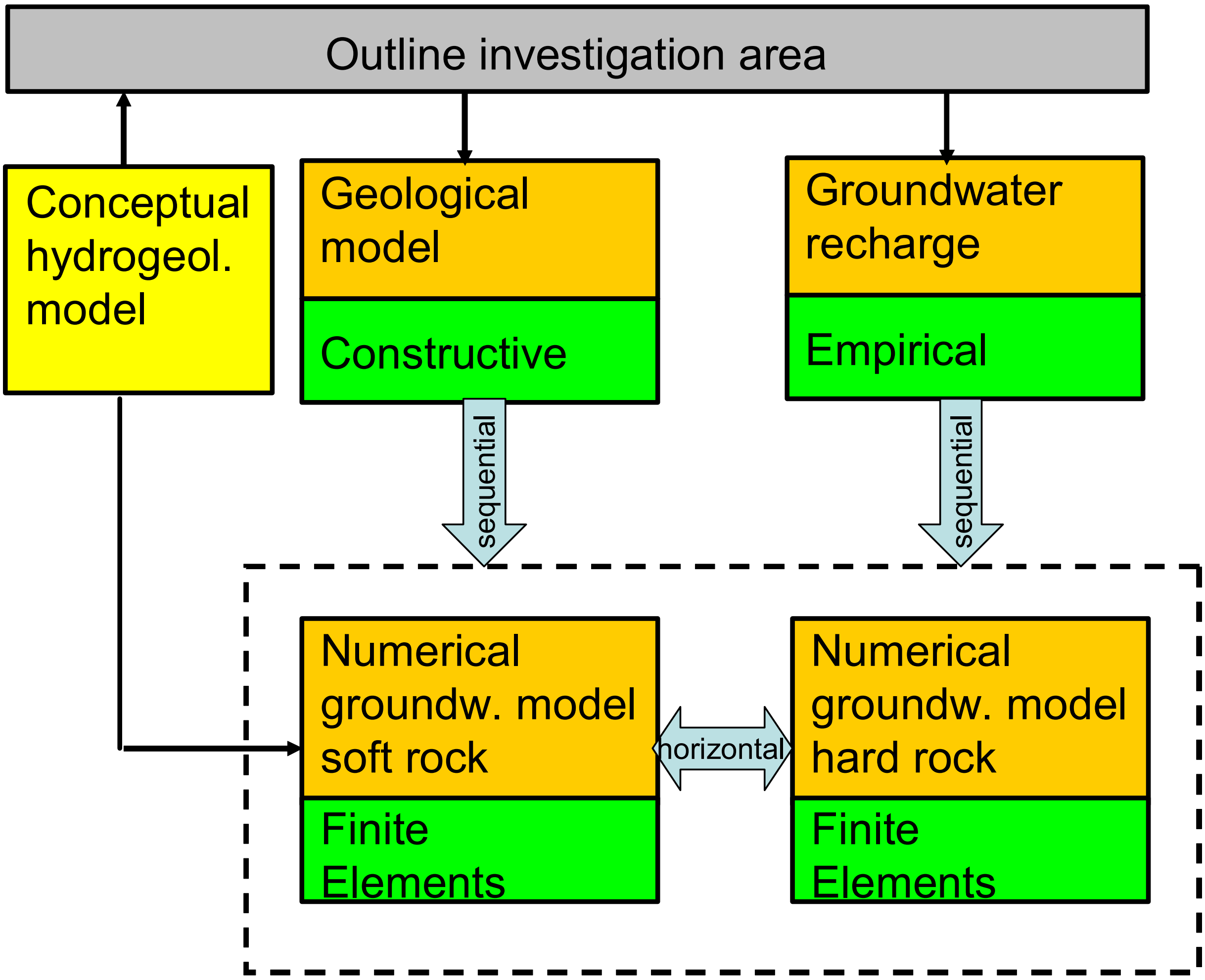


Figure 46: Coupling of the models for the subrosion valley Unterwerra investigation area.

The river Werra was coupled sequentially with the water levels to the numerical groundwater flow model as an internal boundary condition. The water levels were interpolated spatially along the streamline and temporally according to the measurements at some barrages and locks. An iterative coupling of the water budget of the area with the river is not reasonable because the dynamic of the river is dominated by the larger upstream catchment areas.

4.7.2 Nubian Aquifer System

For the model of the Nubian Aquifer System the climatic changes during the Late Pleistocene and Holocene, as presented by PACHUR (1999), were coupled to a numerical groundwater flow model. The "climatic model" is only a transient parameterization of the values for the groundwater recharge including the input parameter for the groundwater model. The assumption of a northward trend of the monsoon to the middle of the investigation area was one of the modeling results. This is not adequate for the modeling approach and does not reflect the results of the investigation of isotopes resulting from very long travel times in the aquifer system.

The hydrogeological structural model was built with geostatistical methods. Databases were geological field investigations. Some rare aquifer tests were analyzed to obtain input parameters for the numerical groundwater model. The porosities were estimated with an algorithm described by SCLATER & CHRISTIE (1980) for oil exploration that corrects the porosities according to the burial depth.

The couplings of these models are shown in Figure 47. In this graphic, the simplicity of the vertical couplings is shown very clearly. The horizontal couplings that were applied by SEFELNASR (2007) make the modeling approach for this area much more complex. These horizontal couplings were not necessary for the long-term model calculated in the context of the impact of climatic changes in the Pleistocene and Holocene.

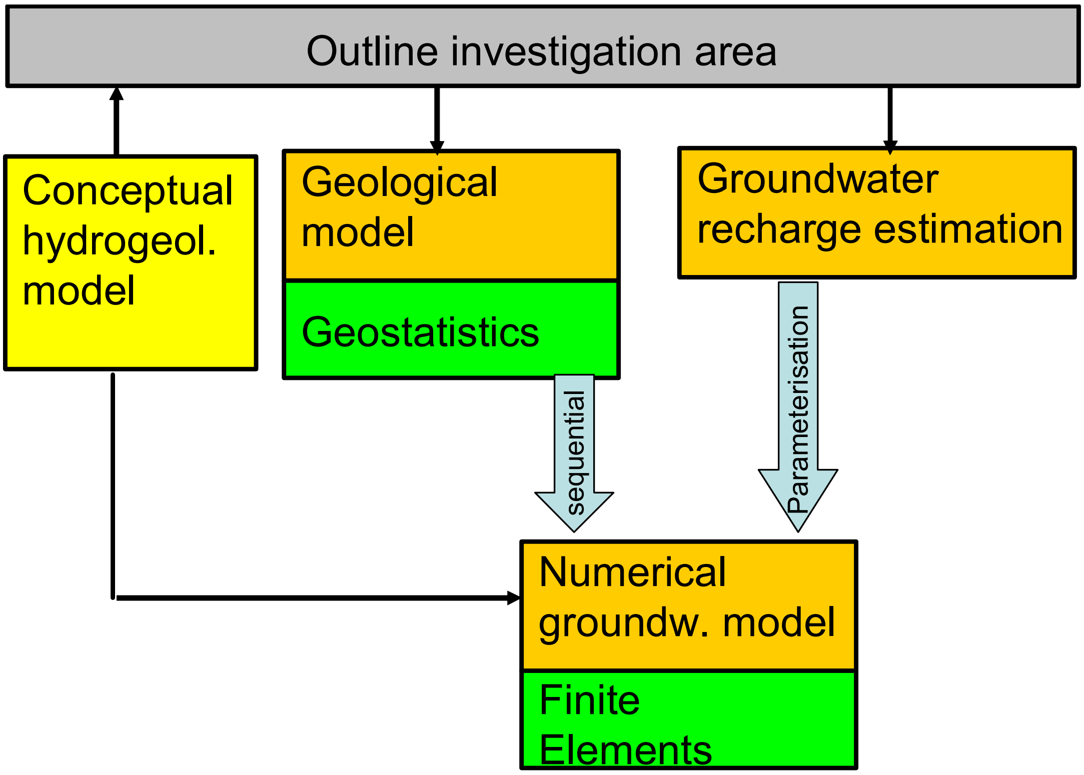


Figure 47: Couplings of the models for geology, groundwater recharge, and groundwater flow in the Nubian Aquifer System model area.

The development areas in the oases were examined using a modeling approach from SEFELNASR (2007) with a highly increased discretization. The interfaces between the areas of low and high resolution were implemented as integrated horizontal couplings. They exhibit slightly unstable behavior.

A different approach to horizontal coupling was used for a more differentiated modeling of the saltwater ingression at the coast of the Mediterranean Sea. This numerical groundwater model initially was a flow model, but in the context of the investigations of the saltwater intrusion, it was connected to a transport model and a density-driven component in the coastal area near the Mediterranean Sea. For the first approach, reported in GOSSEL ET AL. (2010A), the area was only enlarged to the north, and this part was discretized in a higher horizontal resolution. In the second approach, reported in GOSSEL ET AL. (2010B), the former model was divided according to the results of the modeling of GOSSEL ET AL. (2010A), and then a higher vertical discretization with a division of each former layer into five new layers was generated. As expected, this kind of horizontal coupling was more stable than the integrated approach because the coupling was realized without iterations.

4.7.3 Untere Mulde/Fuhne

Several different couplings were used for the very complex modeling task of the Untere Mulde/Fuhne investigation area in order to reach the model objectives and also to compare different coupling approaches.

Horizontal coupling of the geological models

In the (regional) model area Untere Mulde/Fuhne, the detailed geological models of the two central areas were already developed with a resolution of 10 m. After finishing the regional geological model with a resolution of 50 m, the detailed model areas were cut out of the regional model with an additional buffer of 100 m, and the detailed models were inserted. The raster points with the two different discretizations were merged to build the database for a triangulation. This procedure was advantageous – as compared to the method of HUBERT (2005) – in that the original data from the constructive modeling carried out by FABRITIUS (2002) and WOLLMANN (2004) were transferred without changes. The models of FABRITIUS (2002) and WOLLMANN (2004) did not overlap. Furthermore, the edges of the model areas had no significant mismatches for the hydrogeologically relevant units, and thus they were interpolated without problems. The TINs developed from the database of these points were taken as basics for the creation of the groundwater flow model. This procedure was used to achiev a consistent geological model of a horizontal coupling of different static modeling systems. This model fulfills the basic demands of the necessary vertical coupling. After this horizontal coupling of different geological models, this model needed to be converted to a structural numerical groundwater model – a major task in itself.

Vertical model couplings: Infiltration water model and geological data

The infiltration water model was parameterized according to the geological data for the soil parameters. This work was necessary because information about the substrates of the soils was not available for the entire model area. A direct (sequential) coupling with the geological modeling system is only possible for certain geological modeling tools that allow a spatial analysis of the geological model structure based on the DEM. The procedure described above for the analysis of the complete geological model was not possible, because at the beginning of the modeling process for the infiltration water, the geological model was not ready for use. Therefore, in this case study, the simplified version of the adaptation of geological information in the form of a geological map was carried out.

Coupling with climatic models was not the objective of this model, and considering the excessive effort involved in transferring data, this option was not feasible. With some labor and with the help of a certain kind of horizontal coupling, the measurements for the past were available. The modeling of the potential evapotranspiration is fundamentally necessary and can be a solid base for further modeling approaches. Therefore, the coupling to the infiltration water modeling is essential and must be classified as a sequential coupling. The measurements of the rainwater are considered as a parameterization of the infiltration water modeling approach.

Geology and the saturated zone

The workflow for the modeling task showed the central position of the numerical groundwater flow model, and thus this part of the modeling already sets some general conditions for the creation of the regional geological model. The enlargement of the model area was only necessary to obtain valid and stable boundary conditions for the numerical groundwater model. Thus, the regional geological model was used to create structures and to parameterize the numerical groundwater model. To obtain clean structures for the groundwater model, the layers had to be reconfigured to provide a classification into aquifers and aquitards instead of stratigraphical units. Additionally, the according slices had to be proven for intersections, and they were required to hold a minimum thickness for each layer. This procedure is quite complex because the reconfiguration of the layers also involves adapting hydraulic conductivities for the aquifers and aquitards in a spatial distribution and for the inserted numerical layers the values of the over- or underlying hydrogeological layers. The problems were solved with GIS tools in order to obtain the highest available transparency during the modeling process. Another reason is the compatibility of the resulting datasets. This sequential coupling is only feasible for modeling tools with stable solutions to the rewetting problem. One of the modeling tasks is to follow up the history of groundwater extraction according to the history of the open pit mining in this area and its impacts on the groundwater flow and transport conditions. The massive lowering of groundwater levels leads to the drying up of cells in the numerical model. The subsequent cessation of pumping leads to rising groundwater levels a few decades later. If the modeling tool had been restricted to the saturated zone, it would have been difficult to correct the structural model and the parameterisation for nearly each time step.

Models for infiltration water and groundwater

In transient hydrogeological modeling approaches, the coupling of the time-dependent rate of infiltration water (i.e., groundwater recharge) and the numerical groundwater model is a primary reason for the transient behavior and the temporal variability of the groundwater model. The transfer of data for groundwater recharge to a numerical groundwater model is relatively complex because the data are spatially and temporally variable.

The infiltration water rate depends on the depth to groundwater. This leads to an iterative or perhaps integrated coupling according to this exchange value. For the modeling of the infiltration rate, only depths to groundwater of less than 2 m are of interest. For relatively small temporal variations, this input parameter can be regarded as constant but spatially differentiated. Therefore, a periodically synchronized coupling was reasonable and was much more stable than an iterative or integrated coupling.

For the modeling of Untere Mulde/Fuhne, a sequential coupling was implemented first to get a preliminary steady state groundwater model up and running.

For the transient groundwater flow modeling, a periodically synchronized coupling approach was implemented for the major slices that resulted from the open pit lignite mining. Thus, for each of the ten time slices, a new distribution of hydrological response units was calculated based on new calculations of depths to groundwater.

Surface water and numerical groundwater model

The water levels of the river Mulde and a few tributaries were modeled statistically. The dynamical behavior of the surface water is determined by upstream catchment areas of the model area. Therefore, a sequential coupling to the boundary conditions of the numerical groundwater model was suitable. The change of the flow line of the river Mulde that occurred in 1975 made a periodically synchronized coupling necessary.

Coupled modeling of the unsaturated and saturated zone

Modeling of the unsaturated zone was not necessary for the largest part of the model area on account of the small thickness of the unsaturated zone. A first attempt, with a parameterization derived from the soil maps, produced a very unstable behavior. The problem was the distribution of unsaturated layers with a steep water content – water potential curve (van Genuchten curve), especially for the widespread sandy soils. A second approach with smoothly shaped curves was much more stable and could have been used in regards to stability, but these parameter sets did not fit to the observed soils.

The large cones of the draw down near the open pits lead to the necessity of considering of the unsaturated zone in these small parts of the model area. To avoid the above-mentioned stability problems, the interface of the unsaturated zone and saturated zone was implemented using a periodically synchronized coupling between a one-dimensional numerical modeling system for the unsaturated zone and a three-dimensional finite element modeling system for the flow in the saturated zone. This coupling was synchronized according to the time slices of the mining activities. The lithological information and structure that are needed for the parameterization of the unsaturated zone model were derived from the hydrogeological structural model and the geological model. The coupling was carried out such that only the time shift for the input of the groundwater recharge to the saturated zone was calculated. This model coupling proved to be very stable and useful in practice, though it was labor intensive. The three-dimensional unsaturated models are difficult to handle, and an integrated coupling is obviously not suitable when merely the numerical approaches of one dimensional unsaturated flow in three dimensions are used. A coupling (also iterative) of a one-dimensional flow for each numerical cell or node of a three dimensional (saturated flow) model seems to be more successful.

Groundwater flow and transport model of the saturated zone

This coupling was implemented in numerical modeling tools as an integrated coupling. The tools provide the transport modeling systems as an extension of the flow modeling system. The instabilities that arose at several time steps under predictable (but not avoidable) conditions made it necessary to correct the model several times. The reason was that the flow model had already distorted geometries (according to the highly differentiated geology) and thus was unstable because of the cells in the mining areas. For the stability of a coupling, it is very important to account for whether the underlying flow model is steady state or transient. A steady state flow model coupled to a (transient) transport model is generally more stable. In this case, the flow conditions, such as the velocities and boundaries, are already calculated and are not changed during the operation of the model of the transport processes.

The coupling is shown in Figure 48.

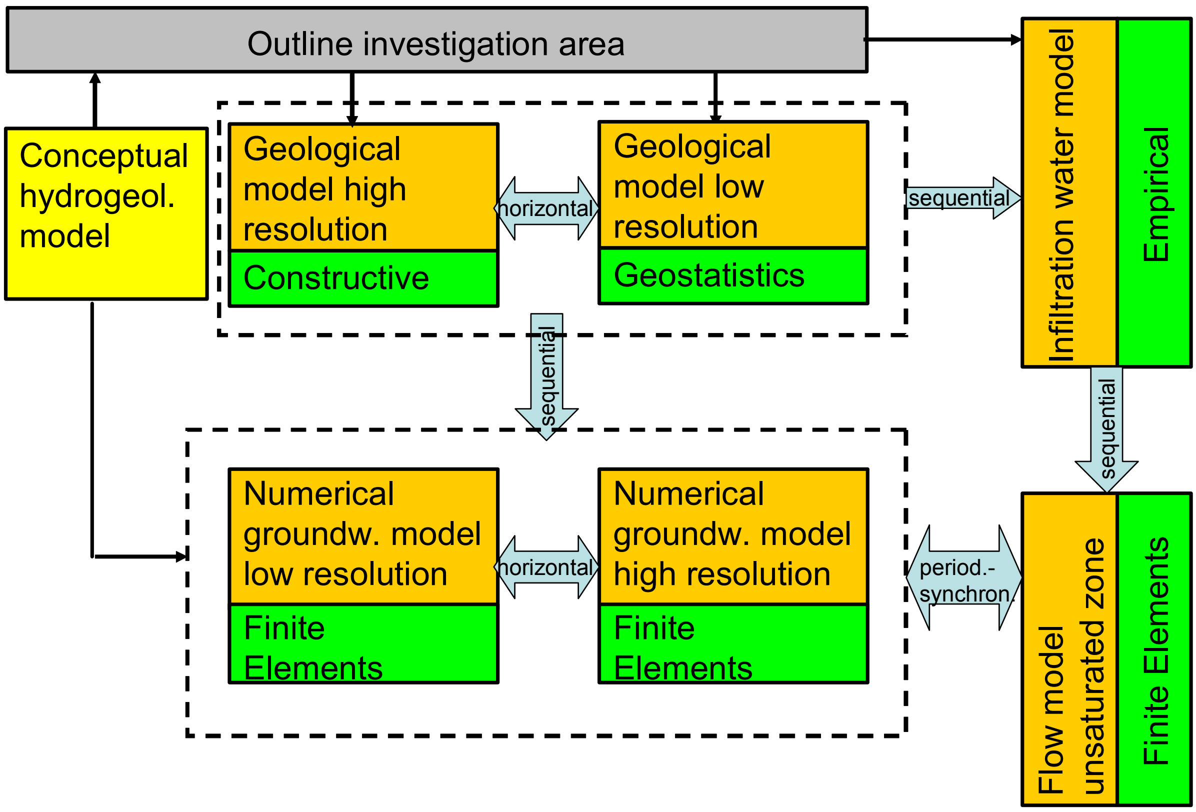


Figure 48: Coupling of models in the Untere Mulde/Fuhne investigation area.

4.8 Summary of the interfaces

For the solution of complex problems, couplings of modeling systems are sometimes necessary. The interfaces for the coupling of modeling systems can be classified systematically. This enables an assessment of the possibilities of the application. The coupling of modeling systems often results in instabilities. As the coupling becomes closer and the connected parameters or boundary conditions become more complex, greater effort is required to stabilize the coupled model. This was demonstrated through case studies of Untere Mulde/Fuhne and the Nubian Aquifer System. Horizontal and vertical model couplings exhibit this behavior to the same extent.

5 Comparisons between coupled models and reality

5.1 Calibration

As a simplification, calibration is described as the adaptation of the model to reality. In the case of hydrogeological and hydrological models, the measured values are water levels and runoff values or flow rates. For geological models, the lithological or stratigraphical description of boreholes must be used. From a theoretical point of view, the process of calibration is a process of systematical changes of parameters of the model function so that a minimum deviation from the objective function (the measured values or derivatives) is reached.

According to BOSSEL (1994), there are several conditions for the modeling approach itself and for the calibration. The behavioral validity (initial conditions of the real and modeled system must match), the structural validity (processes and cause-effect structure of the model must match the structure of the real system), empirical validity (results of a scenario and reality must match), and application validity (model must fit the objectives) should be considered. These conditions are often referred to as verification. They are proven for most commercial and academic modeling systems.

The calibration of models is perhaps the most laborious task in the modeling process and should be performed at the beginning and as part of the objective of the model. In relation to the requirements, the database that must be matched as the objective of the calibration is always insufficient.

The calibration process is very different for the diverse modeling systems. Therefore, the possibilities of single modeling systems are briefly described before the calibration possibilities of coupled models are investigated.

In most of the modeling systems, the use of a parameter estimator is supported. With these tools, the model function is optimized automatically to the objective function by changing only one parameter. In most cases, the parameter variation can be limited so that it will not exceed realistic values.

For the calibration of models, any objective function can be set, but some limits are reasonable. The measurement accuracy of the calibration data is the outer limitation for groundwater levels, i.e. an accuracy of 1 cm at present.

Concerning the deviations of models from reality, some theoretical suggestions will be proposed in advance to fine tune the comparison. BREDEHOEFT (2003) expresses this very dramatically: "My point is that we can choose the wrong conceptual model, fit the data, and get a wrong answer."

A very important criterion for the adaptation may be the question of how expressive are the measurements of the input data or the objective function. As an example, the range of a long-term aquifer test – and accordingly the range of the derived hydraulic conductivities and porosities – is completely different from the range of the determination of hydraulic conductivities from the lithological borehole description or from a grain size analysis of aquifer material. BLÖSCHL (1996) points out that the pure statistical assessment of data will lead to "notoriously poor" results because the main idea behind these methods is the maximum entropy. Geostatistical or – even better – process-oriented analysis methods are much more appropriate, especially for spatially distributed data. Additionally, the characteristics of the measurements must be compared to the parameter distributions resulting from certain processes. As an example, the distribution (and therefore also the necessity of the measurement support) for a fluvial or glacial aquifer differs dramatically from that of a marine aquifer. For this comparison, a geostatistical analysis of the measurements is very helpful because the correlation length of the measurements is determined by a detailed variogram analysis. According to BLÖSCHL (1996), the correlation length is determined by the range of the variogram model. This value can serve as the supported range for the first attempt and it can be compared to the distribution of the measurements. The area of the circle of the supported range r ($\pi \cdot r^2$) can be compared to the area of the Voronoi polygons or Thiessen polygons. If the Voronoi or Thiessen polygons are much larger than the areas calculated from the supported ranges, the support – and also the calibration – is bad. A very exact adaptation of the model to a badly supported objective function is not feasible. A good structured monitoring is an important requirement for the calibration of a model. This is often neglected by authors that focus only on available data in a practical way (OLSTHOORN & KAMPS 2006, HILL 1998, MIDDLEMIS 2001). This method is a minimum condition because it is possible that the real heterogeneity cannot be matched by the measurements at all.

A similar method is reasonable for the analysis of hydrographs or time series data that are needed for a dynamical calibration. In this case, a one-dimensional variogram is calculated first, and then the range of the variogram model is compared to the average time lags of the measurements.

For both methods, spatial as well as temporal, the issue arises as to whether the measurements can reflect the spatial or temporal characteristics of the real distributions. The effect of aliasing in particular must be accounted for to avoid errors in the interpretation.

The question of accuracy demands the calibration of the analysis of the variogram model. In this case, the sill of the variogram model is a measure of the reasonable accuracy. The nugget effect could be suitable, too, but in the case of a distribution where the nugget effect is excluded on account of the assumption of a continuous distribution, this value leads back to the input hypothesis. In addition, the method should be used for the analysis of hydrographs or time series in dynamical models to obtain a more realistic and reasonable argumentation for the objective function in the calibration process. With this method, a better comparison between the hypothetical “measurement distribution“ and the modeled distribution would be possible, as compared to the typically used method of the root mean square (rms) error (SAIERS ET AL. 2004) or the correlation coefficient. The most serious disadvantage of these methods is that they work without an analysis of the spatial or temporal relations.

Calibrations often have the disadvantage of being related to model states for which no real measurement data are available, for a variety of reasons. In these cases, the only way out is the use of proxy data. The biggest disadvantage of proxy data is that their accuracy can be estimated or quantified only very roughly. The case studies will show this in detail for the Nubian Aquifer System and the Untere Mulde/Fuhne model area.

The following paragraphs will discuss which parameters are most suitable for which according objective value.

Infiltration water models

The measurement data for the calibration of infiltration water models are obtained from lysimeters, as described in detail in NEUMANN (2005) and JANKIEWICZ ET AL. (2005). The areas considered in lysimeters are, in most cases, too small for identifying the dependencies of extensive land use variations, e.g. trees or forests. Models can be calibrated with these measurements only under extraordinary conditions because lysimeters are not available everywhere. In most cases, the methods are verified and not the models themselves – not even the results for hydrological response units.

The most sensitive parameters are not easy to identify in the modeling approaches for infiltration water. There are several discontinuous parameters, and the diversity of modeling systems is very high. If the depth to groundwater falls below certain limits most modeling systems react very sensitively. In other modeling systems, the depth to groundwater is not a direct input parameter but rather is derived from the types of the soil and/or the land use.

Unsaturated zone models

Models of the unsaturated zone are much more difficult to calibrate than are infiltration water models because the density of the basic input data is much lower and because the values (input and results) cannot be measured in the same way as the infiltration water amounts of the soil zone in lysimeters. The installation of tensiometers and the calculation of water balances of infiltration rate and the base flow are the only methods of measuring the flow of water in the unsaturated zone below the soil. The base flow is regarded as the amount of rainwater that infiltrated the groundwater, and thus it is considered as the groundwater recharge.

The modeling systems can best be tested in laboratories through column experiments, in the sense of verification.

The parameters are reduced to the saturated hydraulic conductivity and the porosity or field capacity. The boundary conditions are dominant for the modeling because the unsaturated hydraulic conductivity and the saturation of the pores depend on the water infiltrating through the soil.

Numerical groundwater flow models

The calibration of numerical groundwater models is possible for two objective datasets: the water levels, with the comparison of average values of several years, and steady state model results and hydrographs that must be compared to transient model results. The other objective dataset is rarely given but is necessary for all kinds of water flow into or out of the system: the runoff, including the identification of base flow. The latter values are often underdetermined owing to the laborious nature of exact runoff measurements. The method of calibration via the runoff and base flow shows that the objective values for the calibration of models for the unsaturated zone also depend on the behavior of the saturated zone, especially in the case of transient flow regimes.

The definition of objectives for the flow modeling must be defined in accordance with the characteristics of the investigation area. The use of parameter estimators (DOHERTY 1994, CARRERA & NEUMAN 1986) is very interesting and efficient but the resulting model should not be considered to be the best possible model.

Numerical groundwater flow modeling systems depend on the input parameters of hydraulic conductivity, porosity, and the groundwater recharge, which may be defined by some modeling tools as a boundary condition. In some cases, constraints are also possible and/or necessary (see chapter 3.4). This large amount of input data makes the whole calibration process very complex. Some fundamental rules should be mentioned here and should be used in this important task.

The spatial distribution of water levels depends more on the hydraulic conductivities than on the porosities. This part of the calibration thus focuses on those hydraulic conductivities.

The temporal dynamics of water levels are influenced extensively by the boundary conditions. For most parts of the model area, the parameters of porosity/storage coefficient and groundwater recharge are more important in terms of dynamics and budgets.

The statement of SAIERS ET AL. (2004) is very important for the calibration process of groundwater flow models. The consideration of water levels and budgets in combination produces much better results than are possible with the best calibration based on individual objective values.

Numerical transport models of the saturated zone

The consideration of concentrations is the most important database for the calibration of transport models. A calibration via mass balances would be more desirable from a systematic point of view, but the calculation of the objective values is dangerous because mistakes are possible. The advantage of mass balances is the possible comparison of source data with the resulting budgets.

The calibration of the transport model becomes very complex owing to the wide variety of parameters that need to be determined in addition to the advection term. The boundary conditions have systematically the same structure as the boundary conditions in a groundwater flow model, but overall, the transport modeling approach is more complex, especially if several species with their dependencies are also considered. Only the diffusion parameter can be neglected on account of its small variance. For certain substances, this is also true for the biological degradation. The dispersion and sorption processes influence the spreading velocity of substances. The dispersion is more complex than the sorption on account of its scale dependency and the problems involved in measuring the values in the field.

Hydrological models

The modeling of currents in the river course can be calibrated similarly to groundwater flow models through comparison of water levels and runoff values. This is simpler than in groundwater modeling because the measurments are easier, especially for small creeks or grabens. Rainfall–runoff modeling systems spend most of their efforts in the calibration process. The calibration value is the flow velocity, and the parameters are the asperity and perhaps the runoff profile.

Geological models

The geological models presented here and created with statistical or constructive methods cannot be calibrated because they represent only conceptual models in a digital form. The most important difference is that they do not simulate processes.

Based on the available database, the best possible model is created via modeling methods. This model can only be proven in terms of geometrical correctness, i.e., the slices should not intersect. The construction or creation of the model is based on the data that could be used for the objective function of calibration. This contradicts the definition of the calibration. Therefore, the terminology cannot be used for these modeling methods. For process models, the situation would be different because in this case, the geological maps and the borehole data could be used for calibration.

The geological model holds a central position concerning the data support for other modeling systems. Thus, the sensitivity of this data is very high. Therefore, it is very important to evaluate the database in detail. The geostatistical methods described above can be very helpful. Also, at this point, the range should be used for the comparison with the Voronoi-(or Thiessen-) polygons, especially for the application of constructive methods.

Calibration of model couplings

The model couplings described in chapter 4.3 demonstrate the central position of the geological model that cannot be calibrated. The number of parameters transferred to the unsaturated and the saturated modeling system, and perhaps to the infiltration water-modeling system, is comparably small. Carefully planned data handling and processing will encode the parameters via indices to select and change only the selected values in the calibration process. Even the structures will not be transferred without changes, as the figure for the coupling to numerical groundwater modeling systems shows. The indexed processing is very helpful in the coupled modeling approach. Once established, the new structures will not be changed during the calibration; only the values of the parameter setting will be changed. Concerning the geological modeling approach, a question arises: Is it reasonable to adapt a model that cannot be calibrated to another model (created with another modeling system) based on the objective values of this model? This procedure results in an inverse modeling approach.

The modeling gets even more complex if several modeling systems are coupled. The dedicated changes of parameter values can only be handled in a GIS – this is also true for the reconstruction of one of the last parameter sets. Especially for the necessities of a coupling with a geological model, it can be shown that by various points of usage and multiple applications of the derived parameters a high sensitivity must be stated.

Sequential couplings are more labor intensive in the calibration, but they are also more transparent than integrated couplings. Periodically synchronized model couplings fall into the same class, but more effort is required on account of the frequent transfer of values. The calibration of iterative couplings is labor intensive as well as non-transparent. This kind of coupling can only be applied when already well-calibrated models are connected, so that they will not need to be calibrated in the coupled model again. In most cases, integrated couplings support the calibration through a parameter estimator. The number of variables in the more complex modeling systems will increase by this coupling, and therefore the possibilities of the calibration will also increase.

The capabilities and the effort for the actualization are extremely important especially for the coupling with a geological model. Several geological modeling tools allow many possibilities for analyzing the finished model. However, the possibilities for updating have the highest priority considering the calibration process of a coupled modeling approach in which the results of the coupled model are fed back to the geological model. The original task of an update is necessary for importing new information. This is very often not supported by geological modeling tools. In the end, the reason must be sought in the above-mentioned importance of an interactive modeling tool (see chapter 3.1).

5.2 Validation

Validation is used to prove the calibrated model. This should be carried out without a change of parameters (only in certain model constellations) and without a comparison to an independent dataset of measurements (objective values). The boundary conditions – or better the time-dependent data – can be changed according to the conditions at the measurement time step.

The use of model calibrations is assessed differently by different authors. SAIERS ET AL. (2004) and NEUMANN (2005) describe in detail that the validation (post-calibration prediction) resulted in important advances of their models. This is an important step forward in the field of modeling. CARRERA & BASTIDAS (2005) are not convinced of the usefulness of validation from a systematic point of view. The problem of each model, as well as of each scientific theory (a model is an application of a theory), is that it can be verified as often as needed but if there is only one wrong modeling result, it is proven wrong (POPPER 1994). CARRERA & BASTIDAS (2005) estimate the model validation as a kind of reassurance for the modelers. The validation of a model can be better proven for short modeling time lengths. In most case studies, the problem arises for long modeling times when data about the objective values and boundary conditions are not available.

For coupled models, the significance of a validation step is reduced further, because, in most cases, additional parameters must be considered. Those additional parameters rely on sets of an even weaker database, and consequently the possibility of mistakes increases.

Sequential and periodically synchronized model couplings are affected, to a minor extent, if the connected models are validated separately. For iterative and integrated model couplings, the validation of the entire model seems to be much easier than for sequentially or periodically synchronized model couplings, but the parameter internal estimators tolerate much larger error norms, and this results in more unstable models.

5.3 Sensitivity analysis, error analysis, and error propagation

The following chapter on sensitivity analysis does not focus on the sensitivity of the (coupled) models but rather on the effect of the coupling on the sensitivity.

Horizontal couplings are connected mostly by their boundary conditions. The sensitivity concerning these model inputs is very high. Parameters are considered in these cases only in a higher resolution in one of the coupled models. Therefore, only a very general rule must be obeyed, namely, that very high contrasts should be avoided to increase the stability of the total model. A transition area (spatial or temporal) should lead to changed values for the parameters in several steps.

For the vertical couplings, the parameters can differ and vary in a wide range between both modeling systems. Thus, sensitivity analysis of single parameters is nearly impossible in practice. The error analysis is difficult and very complex, even with single models, and the errors cannot be handled with normal physical laws (Gaussian error propagation law). They are more similar to predictive calculations. Instead of changing the dataset of parameters and boundary conditions according to a realistic scenario, the changes are made only for the estimation of deviations. The ranges of the differences based on the changes of boundary conditions and parameters provide feedback for the error ranges of a scenario. When considering only the model coupling, there are only two possibilities for a reaction: either the model couplings increase the deviations and thus lead to divergent behavior of the complete model, or they reduce the reaction of the total model to errors and thus lead to a convergent behavior for the model. There is also the tendency toward unstable behavior of divergent complete models, whereas convergent coupled models are more stable. It is also important that the parameters, initial conditions and boundary conditions contribute to the behavior of a coupled model. The geometries play an important role, especially in three-dimensional modeling approaches.

The analysis of a complete model in regards to convergent or divergent behavior can be carried out with the methods presented in BOSSEL (1994). The disadvantage is that only time-dependent models can be considered. For three-dimensional and time-dependent complex models with highly differentiated input values, this method cannot be used. According to CARRERA ET AL. (2005), the analysis of non-linear systems with typical examples of the coupled models would be possible only via a complete linearization.

5.4 Case studies for the calibration of coupled models

The calibration of coupled models will be analyzed and demonstrated for Untere Mulde/Fuhne and the Nubian Aquifer System in the following chapter. In this chapter, the behavior of the coupling during the calibration process will be considered in detail. The monitoring data of both areas are completely different in spatial and temporal dimensions. In Untere Mulde/Fuhne approximately one observation well for each 1-2 km² is available, whereas in the Nubian Aquifer System only one observation well for every 1000 km² is available. Both investigation areas have a very heterogeneous distribution. The calibration was carried out without a parameter estimator.

An important factor for the adaptation of the spatial distribution is, as stated above, the geological model. In Untere Mulde/Fuhne, a steady state model was calibrated first. This model was coupled only sequentially to the geological model. A first parameterization was achieved based on an infiltration water model and linearly interpolated water levels for the surface water for the boundary conditions. The calibration was made easier through the use of the indication or classification technique for the transfer of lithological descriptions of the borehole data to hydraulic conductivities. The interpolation in one model layer is useful for a reasonable, slight change of values of certain classes. Even this coupled model, which is very easy to use, is not always stable. Distorted geometries of the elements are especially responsible for unstable behavior. In Untere Mulde/Fuhne, the edges of the open pits must be corrected, and the structures of the geological model must be changed. In the Nubian Aquifer System, such changes were not necessary owing to the pure geostatistical interpolations and the structuring according to the limitations of the numerical groundwater modeling system. In addition, for this case study, a steady state model was created first, although it was obvious in both case studies that steady state models cannot fulfill the objectives. The model was adapted to the absolute height of the groundwater level at the observation wells and to the outline of the groundwater contours. The groundwater contours are determined to a certain extent by the hydraulic conductivities in their spatial distribution. In Untere Mulde/Fuhne, an average deviation of 0.38 m was achieved (root mean square of 0.46 m) and the distribution was matched very well.

In the Nubian Aquifer System, the deviation was higher, about I ± 5 m but this was expected for such a large area.

The transient model calibration became much more difficult owing to large gaps in the temporal and spatial distribution of the measurements.

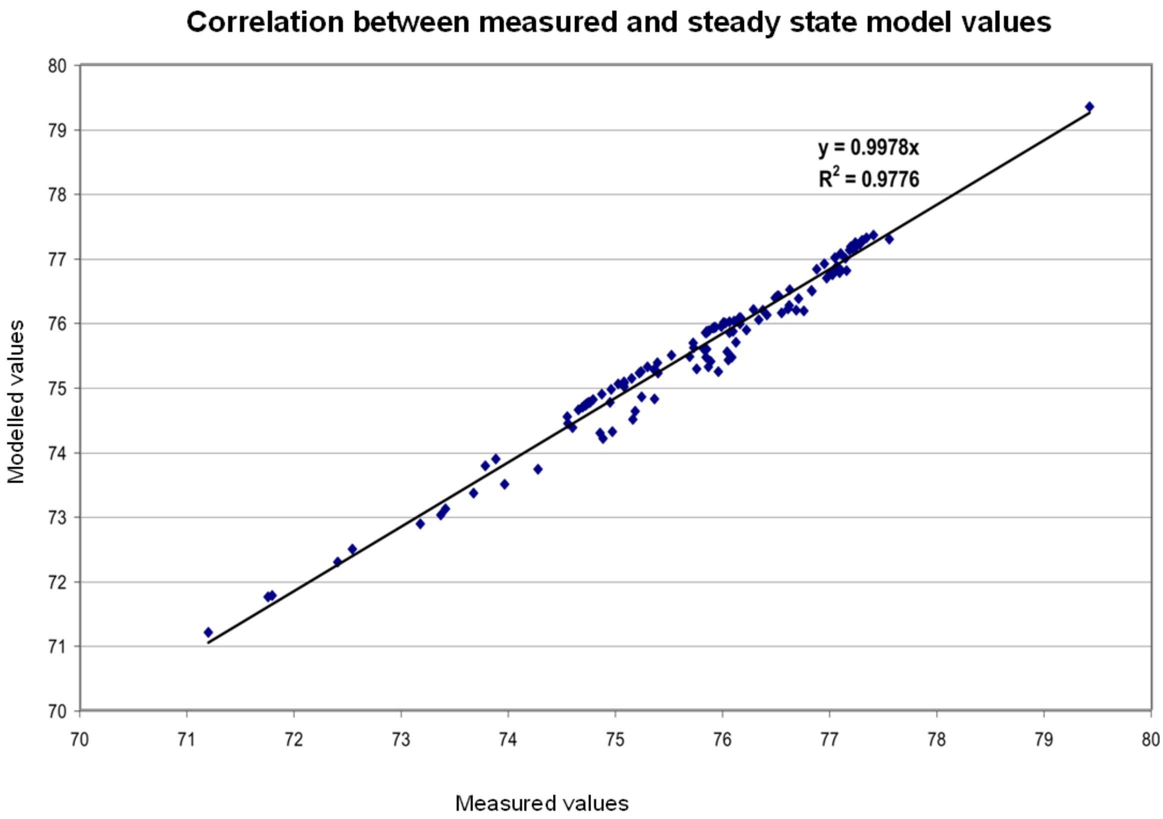
For Untere Mulde/Fuhne, an average groundwater contour map was available for the years 1921 and 1922, and a rough estimation of pumped groundwater volumes (THIEM 1922) was also available. The next report presenting groundwater contours along with a detailed geological analysis was published in the year 1952 (THIEM 1952). Hydrographs for the groundwater were not available for the calibration of the long-term transient model. For a target day measurement in October 2002, the water levels of 142 observation wells were reported. All measurements were located in the area of the detailed geological models. The correlation of these data with the model data was very good, as shown in Figure 49. Additionally, the average groundwater contours for a part of the area from the early 1980s were examined (GROTE & KRÜGER 1984, HELMERT 1984). From April 2005 to April 2006, runoff measurements at a resolution of two weeks for several creeks in the northern part of the model area were available (NEUMANN & WYCISK 2006). This was a valuable source of data for the minimum runoff and consequently for the calibration of base flow and the groundwater recharge. The use of additional data, especially the proxy data from the open pit mining, will be described and analyzed in chapter 6.

For the Nubian Aquifer System, there were only two data sources for calibration: a groundwater contour map from BALL (1927) and proxy data in the form of fluviatile and limnic sediments from the Mid-Holocene.

Calibration with coupled modeling systems becomes – according to the type of coupling – more difficult for transient modeling than for steady state modeling. The sequential couplings are, as expected, relatively simple. Especially after the steady state model calibration, the spatial distribution of the temporally non-affected parameters was established, and it did not need to be changed. The periodically synchronized coupling of the infiltration water modeling was also stable. The calibration of the budget of the groundwater model, calculated via boundary conditions for the creeks in the northern part of the model area, resulted in a good correlation with the measured runoff.

The calibration of the boundary conditions at the surface water bodies was simple owing to the sequential coupling of the statistically elaborated function, and they were very stable in the model's behavior.

For the calibration of the integrated coupling of groundwater flow and transport model for the years 1991 to 1999, hydrochemical measurements were reported (THIEKEN 2001). The determination of the model parameters was somewhat difficult. For the sorption parameters, some investigations were carried out for some locations in the context of a research project (Safira II), but owing to the spatially restricted sampling, the data could not be used for the entire model area. Biodegradation rates were not determined, and this was not acceptable considering the various substances influencing the biological processes. Thus, the transport model was only applied to an ideal tracer. The integrated coupling was very unstable, as pointed out in chapter 4.4. For a first attempt of an analysis of the spreading of substances, neither sorption nor biological degradation was implemented in the transport model. Advection, diffusion, and dispersion were the only input parameters. The results were compared to the concentrations of several substances, and the distributions exhibited high similarity.



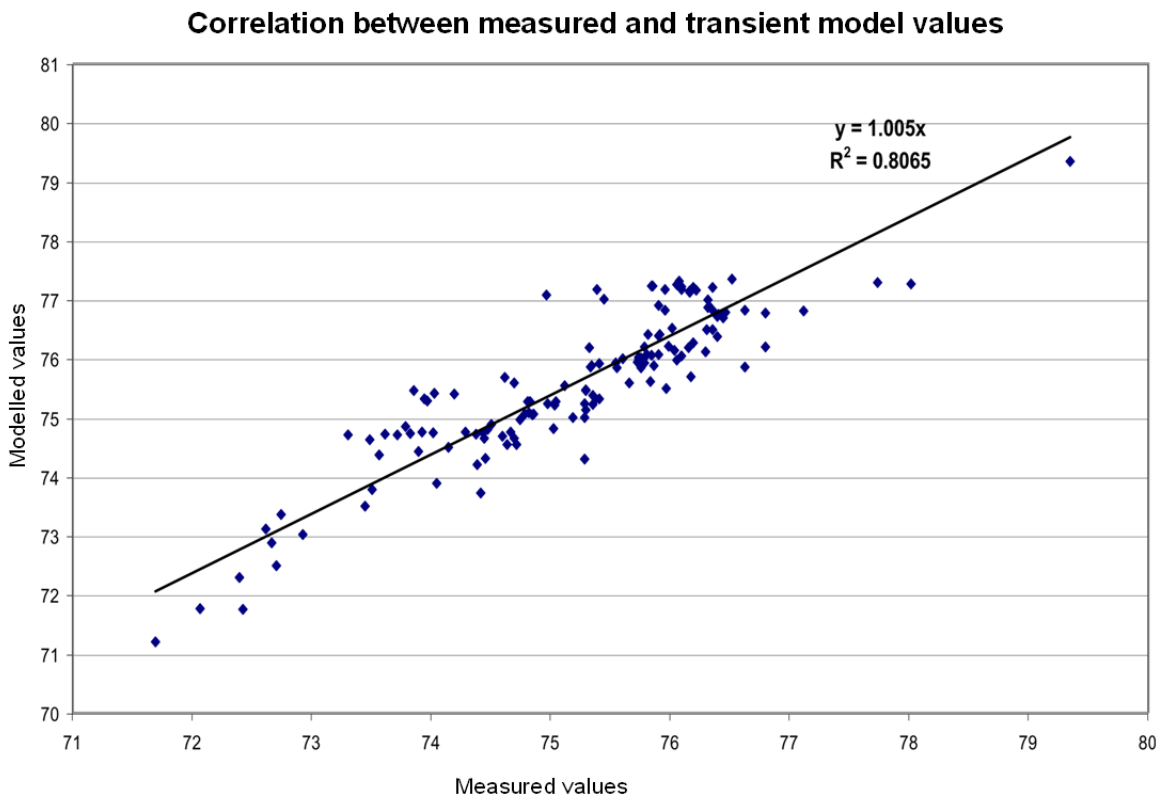


Figure 49: Scatter plot of the measured values and the model data. The linear regression function and the coefficient of determination (0.9776) of the steady state model (correlation coefficient 0.9887) and the coefficient of determination (0.8065) of the transient model (correlation coefficient 0.8981) indicate a very good relation between the datasets (sample size: 142 groundwater observation wells in the Quaternary aquifer).

For the transient calculations of the flow model, the results were slightly worse than those of the steady state model calibration. Although the mean error was only 0.15 m, in no realization was the rms below 1 m (minimum 1.15 m).

The diagram for a calibration of the steady state flow model and the transient flow model shows a high correlation between model results and observed values (see Figure 49).

The comparison of these calibration results with the geostatistical interpretation of the observed data is very interesting. The omnidirectional experimental variogram is non-stationary. For the model area, a trend from southwest to northeast is reasonable on account of the reliable boundary conditions. Considering this direction, the one axis of the resulting ellipse has a sill of approximately 0.2 and a range of 350 m (see Figure 50). Perpendicular to this direction, the range of the axis of the variogram is somewhat longer (400 m). Thus, the Voronoi (or Thiessen) polygons should have an area of approximately 0.5 km². In fact, half of the Voronoi polygons are larger than 0.5 km², as shown in Figure 51, in these cases, therefore, the sampling rate is not sufficient. The mean errors of the calibration results can be compared to the sill, and thus they should be considered sufficiently accurate.

For the Nubian Aquifer System, the groundwater recharge and the porosity were calibrated in the transient model so that the dynamic behavior of a paleolake in the southern part of the model area was matched. The dynamic of the water level of the lake was only available via proxy data (sediments), but the model was able to reproduce the highest water levels, the outline of the area of the lake, and the most probable period in which the lake existed. Thus, the calibration of groundwater recharge and porosity was successful. The saltwater intrusion could be calibrated only according to the outline of the saltwater-freshwater interface as it is observed today.

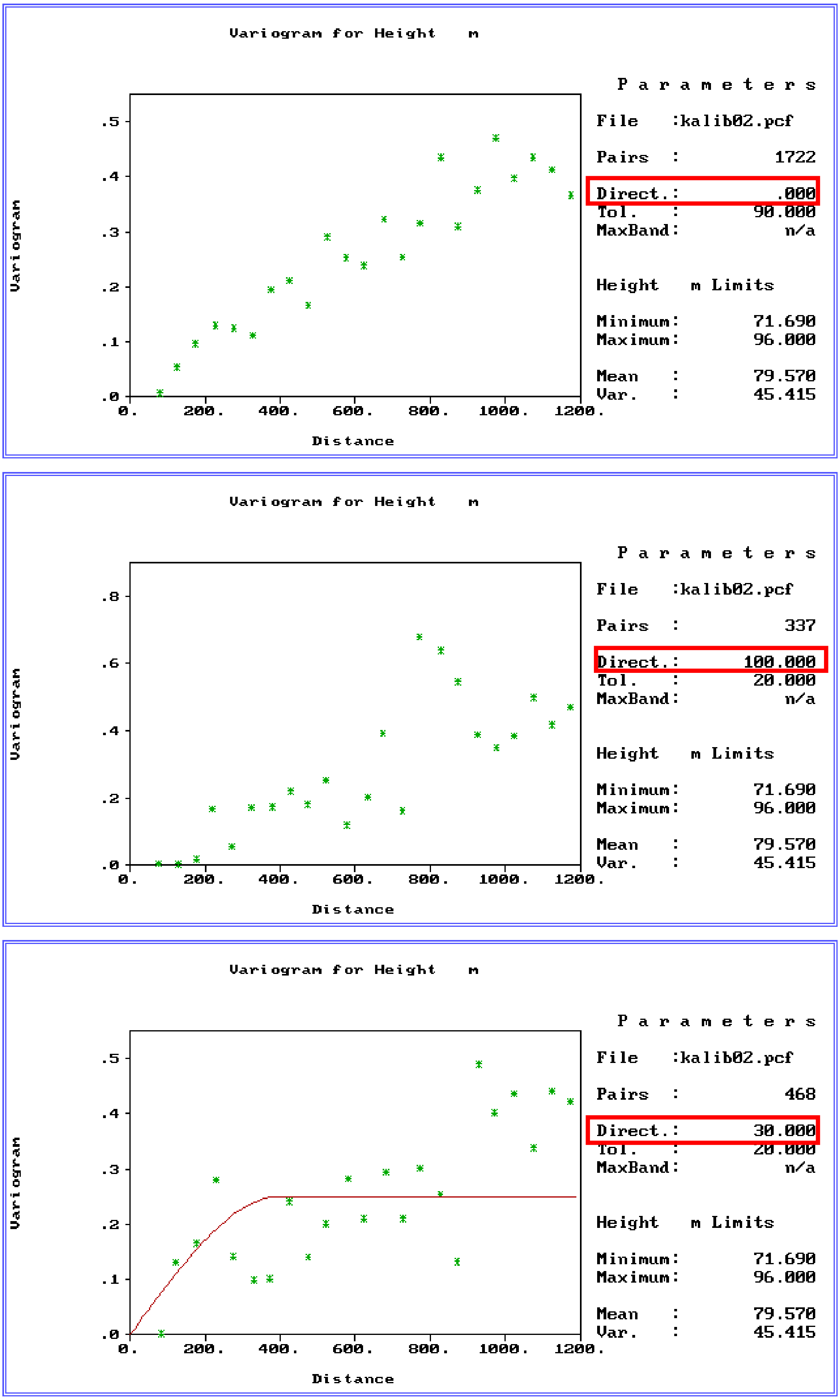


Figure 50: Variograms of the observed data in Untere Mulde/Fuhne for the target date measurement of October 2002. The omnidirectional variogram (top) shows a linear variogram model. Both directional variograms have a sill of approximately 0.2 and a range of approximately 350 m.

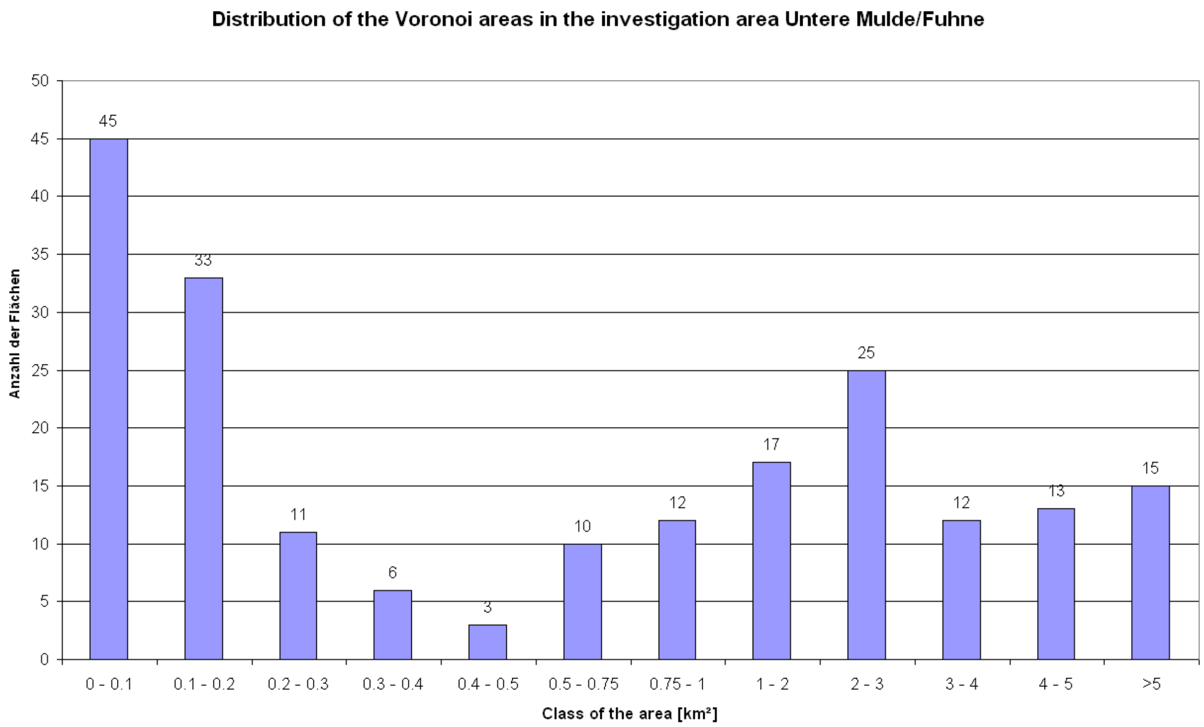


Figure 51: Distribution of the covered area of the Voronoi (or Thiessen) polygons in Untere Mulde/Fuhne.

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5.5 Summary of the model control

The comparison between models with coupled modeling systems and reality is heavily influenced by the type of coupling. Certain types of couplings allow for sensitivity analyses and error analyses only in a reduced range.

6 Predictive calculations with coupled models

The validity of prognoses and predictive calculations in general is discussed very often in relation to diverse scientific disciplines. The modeling methods presented here follow a very mechanical approach in relation to system theory. Only a few statistical methods are used to support the data input or combine to a subordinate extent the combination of methods in the deterministic concepts of the modeling systems. The application of deterministic concepts is thus a prerequisite for all modeling systems presented here, and it can be used in the discussions of prognostic or predictive calculations. With this precondition which is fundamental to the formulation of all single modeling systems considered herein, the couplings and the interfaces are also deterministic. This is an important point in the discussion of the validity and admissibility of prognostic or predictive calculations.

The question of the assessment of predictions is rarely worked out systematically. REICK (2000) presents some methods for investigating the reliability of prognoses. The assessment is carried out primarily with statistical methods to investigate common predictions such as weather forecasts. Predictive calculations of hydrogeological models and model couplings should therefore be evaluated to determine the prediction's accuracy. This can only be done in rare case studies because most of the models are of a purely hypothetical character and are thus never realized – e.g. models for environmental impact assessments and decision support systems.

There is a “golden rule“ in the oil industry for the estimation of the period for a serious prediction: a model calibrated for ten years allows for a prediction of another ten years.

Hydrogeological models are applied very often to the assessment and prediction of impacts on the environment and especially on the water budget. Prognoses are created as scenarios based on calibrated models. The most reasonable way to create prognostic scenarios is to take the parameter distribution of a calibrated model and change only the boundary conditions. A special kind of these prognoses is the “prediction“ of past periods that cannot be calibrated or validated because the relevant measurements are not available. In the case studies for Untere Mulde/Fuhne and the Nubian Aquifer System, such special modeling tasks were necessary.

As pointed out by BLÖSCHL (1996), the change of boundary conditions sometimes must be followed by a change of parameters that should normally remain unchanged, e.g. in the case of a completely changed flow direction of the water for hydrological modeling tasks. Other authors completely deny the admissibility of prognostic calculations of groundwater models because the change of parameters cannot be carried out in accordance with the change of boundary conditions (CARRERA & BASTIDAS 2005).

Because of the importance of prognostic calculations as a task in hydrogeological modeling, the dimensioning and discretization of the model must be fixed according to this task at the beginning of the modeling process. In particular, the choice of the modeling systems, the coupling, and the interfaces of the modeling systems must also focus on the objectives. In development-oriented research projects, this preconditioning does not need to be considered at the beginning.

For the choice of modeling systems for prognostic calculations, the decision about the combination of statistical and deterministic modeling systems is very important. Statistical modeling systems have a disadvantage in that boundary conditions and parameters are summarized without consideration of internal dependencies and connections. Thus, the structural information often is not elaborated adequately and may even be completely neglected. The application of statistical methods in steady state models is thus less critical than in dynamical models. The modeling approach must ensure a proper identification of the most sensitive parts of the model in order to avoid problems with the application of statistical methods.

The possibility of generating a prediction depends on a number of factors:

- Quality of the calibration.
- Predictability of the time-dependent boundary conditions and perhaps parameters.
- Stability of the total model.
- Adequate dimensioning and discretization in time and space.
- Choice of a suitable modeling system.
- Choice of suitable initial conditions for the prognostic calculations.

The method of the coupling of modeling systems plays an important role in relation to the predictability of boundary conditions and the stability of the complete coupled model.

The stability cannot be definitely predicted at the beginning of the modeling process on account of the non-linearity of the system, as shown in chapter 5.3. However, in most cases, with increasing complexity of the complete system, the probability of instability also increases. The probability of unstable behavior can be reduced, as shown in chapter 4.4, by choosing an adequate method for the coupling of modeling systems.

The number of boundary conditions that must be determined for a prognostic setting for future scenarios normally increases with the number of modeling systems contributing to the complete model. The increased number of boundary conditions can also allow for substituting statistical predictions with deterministically modelled values, and this increases the reliability of the prediction.

The following case studies demonstrate these effects of modeling approaches in special cases of prognostic modeling. For these case studies, models are not calculated into the future but into the past using accordingly changed boundary conditions. These models are calibrated as usual for recent measurements. The advantage of this method of proving theories is that proxy data are available for several system stages.

In the case study of Untere Mulde/Fuhne, the groundwater recharge was set for the first model of the groundwater models (the steady state model) by a pure parameterization according to the climatic conditions in the calibration year with a spatial distribution. This method of recharge calculation was replaced in the transient groundwater models by a time-dependent modeling of the infiltration water with a monthly resolution. The empirical calculation of this boundary condition or parameter is much easier and more reliable than the pure estimation. Another example is the interpolation of boundary conditions of first kind (predefined water levels) that was supported by the results of a time series analysis. In this case, the function was assembled by a periodical function and a flooding event in each year. In addition, this procedure substitutes for an estimation of water levels and results in a higher reliability of the complete model.

A special challenge of the Untere Mulde/Fuhne model is the modeling of the pumping of groundwater for the open pit mining. There were only single and very rough data for the groundwater extraction, and these data were not suitable for a direct implementation in a groundwater model. The only source of proxy data was the bottom of the lignite layers from the Miocene. For the mining activities, the water levels had to be held below this depth. The “prognostic” calculation resolved this issue with a special kind of calibration that fit the pumping rates to the necessary depth derived from the geological model. As a result, the typical “traveling” of the cones of groundwater extraction in this region can be observed. This process influences the transport model directly through a corresponding spreading of the infiltrating substances. In addition to the extraction patterns, the geological model – with some dominating features such as fluvial or subglacial channels – plays an important role.

7 Forecast of further developments

It can be foreseen that in the future development of modeling systems vertical couplings of parts of the water cycle will be increasingly important. This will occur independently of the obvious modeling tasks, namely, the modeling of natural or anthropogenic impacts. In some modeling systems, the approaches to pre-emptive development have already been prepared. Other modeling systems must be enhanced and updated in order to obtain better results for the modeled compartment. It is of minor importance whether this is reached by a direct integration of additional modeling methods or by a modularization. This process depends to a certain extent on the development of computer resources and on the demands of the users. The development of coupled systems can result in either increasing complexity of the modeling systems or severely increasing demands on the parameters. Therefore the modeling systems are more problem and data oriented and provide more flexible solutions in the end.

The development of geological modeling systems benefits from the enhancements of visualization possibilities from new developments, e.g. in the context of 3D visualization. From the point of view of statistical or constructive modeling methods, there is an urgent need to enhance not only the visualization capabilities but also the capabilities for an interaction that handles the methods adequately. The current arising problems in the data exchange of highly specialized software tools for geological modeling and their visualization in caves or using special 3D displays will certainly be minor problems that can be solved either in the context of some modeling tasks or, in a more general way, in a collaboration among the most specialized companies. Interaction goes far beyond these most obvious development tasks – it means the possibility of visualization and change of the elaborated models in real time. Additionally, the database for the set up of high-resolution models is currently often inadequate. The geological surveys must provide additional information to increase the data quality and the number of investigations. Enhanced investigation methods may also need be developed.

For the future development of hydrogeological modeling systems, it can be foreseen that the numerical solutions for the saturated zone, as well as for the unsaturated zone, will be applied to an increasing number of problems. The resolution and the dimensions of the model areas will increase according to the higher computer capacities in memory as well as in computational power. The modeling of groundwater flow and transport at a regional scale will be supported by these developments. This trend in development is impeded by the deficiency of data that are reliable enough and that have a sufficiently high spatial resolution for the parameterization of the numerical models. The present spatial resolution of approximately one borehole per km² is not suitable for regional models that work with a locally higher resolution. Additionally, reliable methods for the determination of hydrogeological parameters should be introduced into more geological investigation programs. This is most important for the determination of transport parameters. These parameters in particular are very difficult to determine.

For the modeling of infiltration water and, to a lesser extent, for the modeling of the unsaturated zone, the task is completely different. For these modeling systems, the modeling techniques play a minor role. The present methods must be connected to one single preferred method; the recent calibration technique of comparing the results of different modeling tools with each other must be replaced by a single comparison with adequately recorded field data. A future problem will arise from the lack of adequate data, but not – as in the case of geological data – with a higher spatial resolution. Most important for the future will be the acquisition of completely new kinds of data, such as the leaf area index (LAI), climatic parameters, and parameters for the root zone. Otherwise, the development of modeling methods will cease with the application of empirical formulas. For a real deterministic process modeling, additional processes have to be regarded.

Owing to the increased interest in recent hydrological developments with floods and droughts, the databases and measurement methods in hydrology have undergone rapid development, so that in this field, the requirements for data will be covered according to the recent modeling objectives in the near future. The modeling methods will perhaps change from the presently used statistical methods to numerical methods that reflect the system behavior in a better way. This will enhance both the physical modeling approaches for adequate process modeling and the system analysis and modeling of regional catchment areas. The data exchange for the application in terms of the EC water directive is a step toward this overall objective and has already had (and will continue to have) a direct and positive influence on data availability for regional projects.

For modeling in environmental geology, the perspectives on development are very diverse. The modeling systems and tools of hydrochemical equilibrium reactions are already in a very advanced state in regards to water-rock interactions. For these modeling tasks, the demand and the research projects for a better database will develop according to the applications in projects. An enhancement for environmental impact questions is most important for the future of these modeling systems. This can be seen in the most recent developments in research and applied projects. This concerns both research into the terms of biological and ecological receptors and the implementation of non-equilibrium reactions and reactions with very low velocity.

Considering the diverse possibilities of model couplings, trends can be assumed from their applications and from the systematic investigations. These trends are directly related to the development of the modeling systems that contribute to the coupling.

Horizontal couplings will decrease in importance as a result of new numerical calculation methods and higher computational power. In the near- and mid-term future, they will be necessary for enhancing some modeling tools to fulfill the increasing demands for high-resolution information and modeling results. This affects especially the modeling systems for the saturated and unsaturated zone that work with numerical methods. Static geological modeling systems will certainly not face these changes because they do not depend on high computational power. For the modeling of infiltration water, the described development of new methods will not be more rapid than the evolution of computational capacities.

For vertical modeling couplings, different trends of development should be considered. For several modeling tools, diverse strategies are developed for the integration of additional modeling systems. This enhances the application of recent scientific methods. In these tools, the user does not need to think of exchange formats or additional parameterizations, and thus the work becomes simpler. On the other hand, the integrated vertical couplings will become unstable very rapidly. The connection of different modeling systems will become simpler on account of future enhancements of the data exchange formats. A central position will be taken by GISs. This role is nearly the same as in present modeling approaches. Additionally, the database management systems will provide enhanced data exchange. The proprietary and undocumented formats of several commercial producers will become useless in the future. Thus, some recent developments in commercial GIS tools will not support and enhance modeling in the future. Some important approaches to open formats that will simplify the development of interfaces are now implemented in the OpenSource tools.

For many users, the present trend of implementing internal interfaces in the modeling tools helps much more than does the integration of new modeling systems. Some modeling tools are already internally constructed using modules and as OpenSource tools, and they do not need an opening such as other tools. The users can define the kind of coupling on their own with this capability, and thus they can adapt the complete system adequately to the problems that need to be solved. Whereas the integrated and iterative couplings tend to become unstable, the easy-to-use interfaces of the tools can help to stabilize the system behavior. Stabilization is achieved through sequential or periodically synchronized couplings for critical complex systems. The possibility of using a modeling system that best fits the modeling task is an additional advantage. This coupled modeling system can be chosen and adapted by scientists according to their skills, the database, the basic knowledge, the requirements, the contract with the client, etc.

The increased application of coupled modeling has several consequences for the workflow and working techniques. This may cause some problems, as described in the following statements:

- The requirements for scientific techniques and knowledge for users of coupled systems far surpass those for users of a single modeling system. Owing to the increased complexity of the modeling systems, the expectation of simpler and more user friendly modeling tools for prognostic calculations cannot be realized in the near future. This means that when using complex models, teams of scientists must work together, especially for the most important steps in the workflow of the models, such as the configuration and the maintenance. Predictive calculations will require much more knowledge about the connection of modeling systems than is necessary with single modeling systems owing to the complex definitions of scenarios.
- The database will become the bottleneck of prognostic calculations on account of the diversity of parameters and the necessary spatial and temporal resolution. In most cases, remote sensing data and new field methods or exploration methods will reduce the severity of the problems, but new demands for data storage and handling will arise. The systematic extension of storage capacities and computational power will require state-of-the-art computing capabilities. The new possibilities related to parallel computing are very interesting for the application of many modeling systems coupled by periodically synchronized – or in some cases iterative – coupling approaches. These opportunities for the development of hardware should be recognized in the design and improvement of current modeling systems.

The applications of vertical modeling couplings will undoubtedly proliferate in the future. In these approaches, not only the described modeling systems but also the connections to biological and technical modeling systems play a role. Additionally, their success will depend on collaboration among scientists of diverse disciplines who are able to handle a variety of modeling tools and their connections and interfaces in proper technical and scientific ways.

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