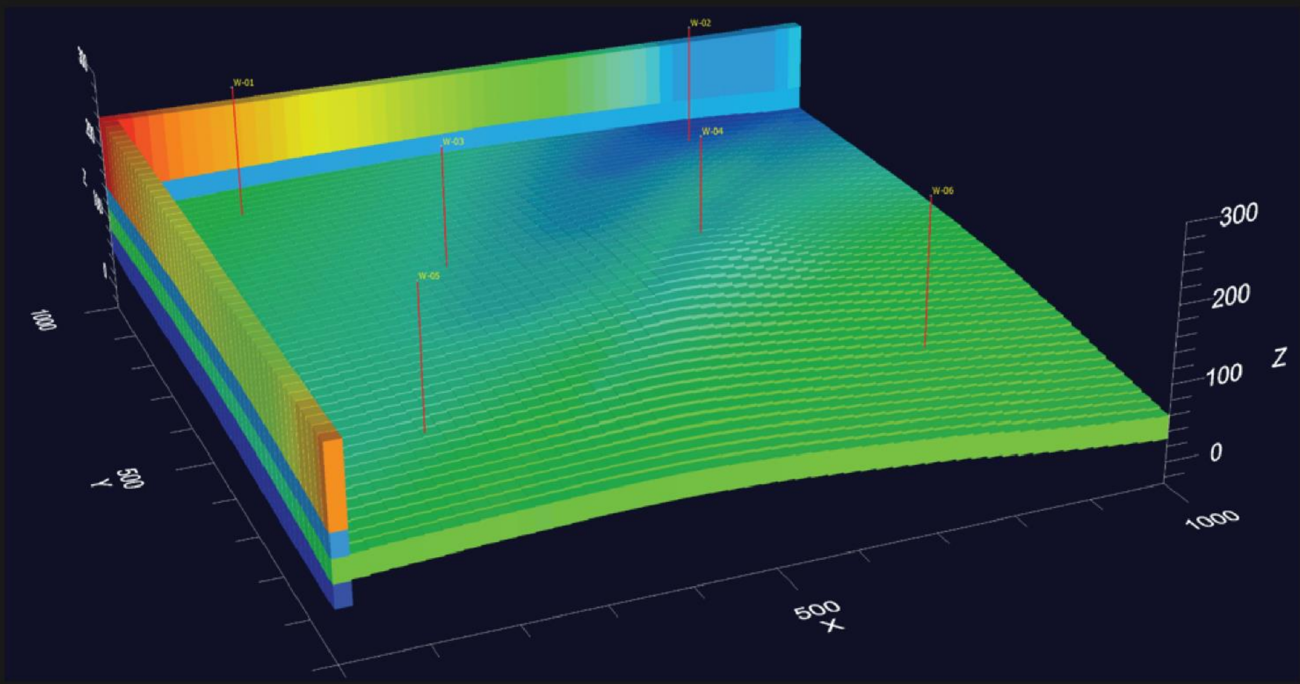

Geologic Frameworks for Groundwater Flow Models

J.P. Brandenburg

THE GROUNDWATER PROJECT

Geologic Frameworks for Groundwater Flow Models

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J.P. Brandenburg
Senior Geologist
Haley & Aldrich, Incorporated
Ann Arbor, Michigan, United States

Geologic Frameworks for Groundwater Flow Models

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THE GROUNDWATER PROJECT

Cover Image: J.P. Brandenburg, 2020

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The Groundwater Project Foreword

The United Nations Water Members and Partners establish their annual theme a few years in advance. The theme for World Water Day of March 22, 2022, is "Groundwater: making the invisible visible." This is most appropriate for the debut of the first Groundwater Project (GW-Project) books in 2020, which have the goal of making groundwater visible.

The GW-Project, a non-profit organization registered in Canada in 2019, is committed to contribute to advancement in education and brings a new approach to the creation and dissemination of knowledge for understanding and problem solving. The GW-Project operates the website https://gw-project.org↗ as a global platform for the democratization of groundwater knowledge and is founded on the principle that:

"Knowledge should be free and the best knowledge should be free knowledge." Anonymous

The mission of the GW-Project is to provide accessible, engaging, high-quality, educational materials, free-of-charge online in many languages, to all who want to learn about groundwater and understand how groundwater relates to and sustains ecological systems and humanity. This is a new type of global educational endeavor in that it is based on volunteerism of professionals from different disciplines and includes academics, consultants and retirees. The GW-Project involves many hundreds of volunteers associated with more than 200 hundred organizations from over 14 countries and six continents, with growing participation.

The GW-Project is an on-going endeavor and will continue with hundreds of books being published online over the coming years, first in English and then in other languages, for downloading wherever the Internet is available. The GW-Project publications also include supporting materials such as videos, lectures, laboratory demonstrations, and learning tools in addition to providing, or linking to, public domain software for various groundwater applications supporting the educational process.

The GW-Project is a living entity, so subsequent editions of the books will be published from time to time. Users are invited to propose revisions.

We thank you for being part of the GW-Project Community. We hope to hear from you about your experience with using the books and related material. We welcome ideas and volunteers!

The GW-Project Steering Committee

November 2020

Foreword

Applied hydrogeology requires application of conceptual models to represent the conditions for groundwater flow which are key to solving groundwater development and contamination problems. Understanding groundwater conditions begins with understanding geology and using that geological information to estimate hydraulic conductivity and porosity. In turn, the distribution of hydraulic conductivity and porosity inferred from geologic information are used to create hydrogeologic representations of a groundwater flow system. Prior to the 1970's, this conversion was accomplished using pencil and paper but now it is done using readily available software. However, to use the software effectively, it is essential to understand this conversion process. This book: Geologic Frameworks for Groundwater Flow Models by J.P. Brandenburg is an introduction to the conversion process that has become well established in the petroleum industry but has lagged behind in the hydrogeology industry. Hydrogeologists know that three-dimensional numerical flow models are essential, but it is the conversion from geologic data to the hydrogeologic model that needs clearer recognition. This conversion is known as: 'static modeling', which is the precursor to 'dynamic modeling'. Dynamic modeling refers to the flow and transport modeling (i.e., aquifers do not move so are static, but the fluids are in motion so are dynamic).

J.P. Brandenburg, author of this book, is exceptionally qualified for the task because he is extensively educated in both geology and fluid flow; has undertaken conversions for sophisticated static and dynamic modeling in the petroleum industry; and currently is focused on conversions for complex three-dimensional groundwater models.

John Cherry, The Groundwater Project Leader

Guelph, Ontario, Canada, November 2020

Preface

Groundwater modelers should be familiar with and have access to systematic methods for translating physical subsurface geology into a numerical representation. Other hydrogeologists will benefit from understanding the process. This book introduces techniques for creating the underlying geologic framework of groundwater flow models. It is arranged around a hypothetical site with contaminated groundwater, beginning with a discussion of data collection and geologic interpretation, then delves into the steps required to build a realistic numerical model. The reader will find that many of the methods and calculations can be applied with tools as simple as paper and pencil. Links to publicly available computing resources are provided where possible.

Acknowledgements

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The suggestions and contributions of Eileen Poeter are appreciated. I am grateful for the oversight of Amanda Sills and copyediting of Elhana Dyck, both of the Groundwater Project, Guelph, Ontario, Canada. I thank Eileen Poeter (Colorado School of Mines, Golden, Colorado, USA) for copyediting, layout editing and production of this book. The cover figure was generated using Visual MODFLOW Flex software from Waterloo Hydrogeologic.

1 Overview

A model of subsurface geology is needed before simulating groundwater flow. The petroleum industry has had better defined procedures for geologic modeling than the groundwater industry, so the Ground Water Project provides this book to review the basic process of subsurface modeling including techniques from both a groundwater and petroleum perspective. Given the commercial interests of the petroleum industry, attention is focused on accurately simulating the volume, flow and extraction of fluids from the subsurface. The techniques described in this book, in particular the concepts of *net thickness* (the thickness of coarser-grained strata that support fluid flow) versus *gross thickness* (the total vertical thickness between bounding units), are not only important to petroleum production, but also relevant to simulating groundwater fluxes, which can be of interest to water resource modelers who are estimating storage volume in aquifers.

Numerical models constructed to simulate contaminant fate and transport require more detailed delineation of geology. For such applications, the distribution of heterogeneous geological properties is needed because contaminants follow preferential paths through connected high hydraulic conductivity zones and many fate and transport processes depend on the interchange of fluids with differing chemistry between zones of differing hydraulic conductivity.

Modeling techniques presented here pertain only to clastic aquifers, which are composed of sediments or sedimentary rocks derived from mechanical weathering, basically some combination of gravel, sand, silt, and clay. These may be unconsolidated (loosely packed, uncemented grains) or consolidated (tightly packed, cemented grains). These techniques do not apply to fractured bedrock, karst, or other aquifers where secondary porosity is the dominant flow pathway.

The groundwater software Visual MODFLOW FLEX↗ from Waterloo Hydrogeologic is used in this book. It is a software program that facilitates groundwater flow modeling with the most commonly used groundwater flow simulation tool: the USGS MODFLOW code↗. It also has the advantage of sharing some ancestry with Schlumberger's Petrel software, an oil and gas industry standard for subsurface geologic modeling. The RockWorks↗ geologic modeling software is also used in this book. It is used to generate a distribution of geologic materials that can be assigned hydraulic properties which are then converted into values for a groundwater modeling grid such as one defined by MODFLOW.

2 Introduction

Hydrogeologists work with other geologists and engineers to develop a framework that provides the basis for defining the properties of a groundwater flow model in a two-step process; static modeling followed by dynamic fluid flow modeling.

Unchanging properties of the geology are characterized in the static model, while the dynamic model simulates flow and adjusts hydraulic properties if changes in the flow system alters the properties.

For example, declining pressure during fluid extraction causes geologic materials to compact, reducing hydraulic conductivity and porosity (dynamic properties). Meanwhile, the amount of sand relative to shale in the reservoir will not change (a static property). A static model is built using geometric tools and is used to populate a flow simulator with hydraulic properties. A dynamic model is built using a flow simulator (for groundwater, MODFLOW is commonly used) and is used to adjust hydraulic properties by matching the simulation with measured data from the field so that the simulator will reasonably predict changes in the flow system in response to stresses. Traditionally the static model was developed by geologists then handed over to the engineers for dynamic simulation. However, experience has shown that this one-way process has some limitations as the calibration of the dynamic model can provide additional insight into the geology, and understanding of the geology can constrain the parameters required for calibration. Today the process tends to be more iterative. In the groundwater industry the modeler is often skilled in mathematics, engineering and geology, or a group of experts work together to develop the model.

Building groundwater models tends to be a geographically intensive process, with attention on map-view details and simplification of the subsurface into a series of aquifers or hydrostratigraphic flow units. This is certainly the most appropriate approach to regional or watershed scale modeling, and many sophisticated GIS tools are available for such work. However, these tools and methods can be cumbersome when dealing with site-scale models, which may have an area of only a few thousands or hundreds of square meters.

This book focuses on building contaminated-site-scale groundwater models using workflow concepts employed for static modeling of petroleum reservoirs. No particular software programs are advocated, as a large part of the work can be done with paper and pencil or generic contouring software. Many of the core concepts pre-date modern computers with graphical capability and haven't changed with improved software.

The static modeling workflow is presented here as a series of steps building a model for a hypothetical contaminated site (the Test Site). This starts with the thought exercises needed to build a useful conceptual model, moves on to techniques for transforming the conceptual model into a three-dimensional (3D) numerical model, and culminates in the process of using the framework to create a flow model.

3 Context and Purpose

Before beginning any modeling project, the goals of the project should be clearly defined. Useful evaluations of flow and transport can be undertaken using analytical models, often via a spreadsheet. It is good practice to start with pencil and paper and see how many questions can be answered before building a complicated numerical model. If nothing else, careful calculations provide a baseline to evaluate the basic functionality of future, more complex models.

3.1 Conceptual Models

Most environmental projects for contaminated groundwater sites are required to prepare a conceptual model in order to comply with government regulations. The conceptual model defines basic details of the contaminated aquifer; its geometry, depth, thickness, range of hydraulic conductivities, observed hydraulic heads, and features of the system that influence hydraulic behavior such as surface water bodies and pumping wells. For smaller contaminated sites, it is likely that the details of the conceptual model are adequate to meet regulatory requirements, but do not provide sufficient detail for the modeling to effectively predict the behavior of the system, and thus to design the remediation plan. Conceptual models that describe thick layers with homogeneous properties are an indicator that more thorough review may improve the model.

3.2 Local Geology

Familiarity with local geology is a necessity for any subsurface modeling. Boreholes for water supply wells, geotechnical investigation, and other applications are abundant, often with publicly available logs and published interpretations. It is useful to review reports from other groundwater projects in the area to glean information about subsurface properties and conditions, and to learn from problems encountered by others doing similar work.

3.3 Structural Geology

The data required to identify structural geologic features are essential but not sufficient for many contaminated sites. Consequently, faults may not be identified, and the bedrock surface is often characterized as a monotonic flat surface or typical depth, while in actuality it may have a complex topography. The bedrock surface is extremely important at sites with dense non-aqueous phase liquid (DNAPL) contaminants because the DNAPL sinks to low permeability layers and further migration is controlled by the topography of the surface. Faults can be found virtually everywhere in the world. For example, areas of the Texas Gulf Coast are affected by surface deformation related to creeping faults although that part of North America is tectonically quiet. Often small faults are identified at contaminated sites by noting locations of steeper hydraulic gradients. The Test Site example presented in this book contains a small normal fault.

3.4 Stratigraphy

The sparsity of data at contaminated sites also presents challenges to delineating the stratigraphy. However, more stratigraphic data has been collected in recent years as often stratigraphic complexity is proving to be a key limiting factor to successful remediation. Remediation methods that involve extracting and injecting groundwater can be limited by baffling of flow by low permeability stratigraphic barriers. Thin layers of fine-grained soils rich in clay and organic matter can have a high capacity to trap groundwater contaminants. After the more permeable portions of the aquifer have been remediated, these contaminants can diffuse back into the clean groundwater, causing an unexpected rebound in concentrations. Layers like this can be easily missed using older technologies such as auger and rotary drilling. Electronic borehole logging and high-resolution direct push sensing tools can be used to create logs with the necessary level of detail. However, stratigraphic principles are required to make a meaningful determination of how these details extend into the space between boreholes. Guidance documents such as Schultz et al. (2017) contain detailed information and workflows on how to make such stratigraphic assessments.

For oil and gas reservoirs, much characterization is done by considering and comparing sedimentary depositional facies (e.g., Shepherd, 2009). For example, the relative homogeneity of aeolian (sand dune) facies leads to better reservoir connectivity than the layered and highly dissected nature of deep-water channelized turbidites. This topic is worthy of its own textbook and is not discussed here except to say that environmental projects can benefit from the same line of inquiry. Again, contaminated groundwater sites are often of limited extent or the funding to collect the necessary data is lacking, rendering such stratigraphic analysis impossible.

4 Building a Framework

The geometric framework is the foundation for static modeling. This orients the contaminated site in three dimensions relative to the defining boreholes.

4.1 Maps and Cross Sections

For many years, maps and cross sections formed the entire framework for static modeling. With modern computer software, this is now done in immersive 3D environments that facilitate spatial conceptualization. However, maps and cross sections still underpin the 3D interpretations in many ways. For this example, traditional maps and cross sections are used for the interpretation.

The Test Site is approximately 9 hectares in size and has been characterized by 14 boreholes. The boreholes are arranged in two roughly perpendicular transects and were drilled through unconsolidated sediments and terminated at the top of bedrock. The ground surface is between 70-73 meters above sea level, and slopes towards the south. Bedrock was encountered at depths ranging from 40 to 70 meters below ground surface. The geometric details used to construct the interpretation framework are shown in Figure 1 where the two cross sections have been arranged immediately next to the map, with everything drawn to scale.

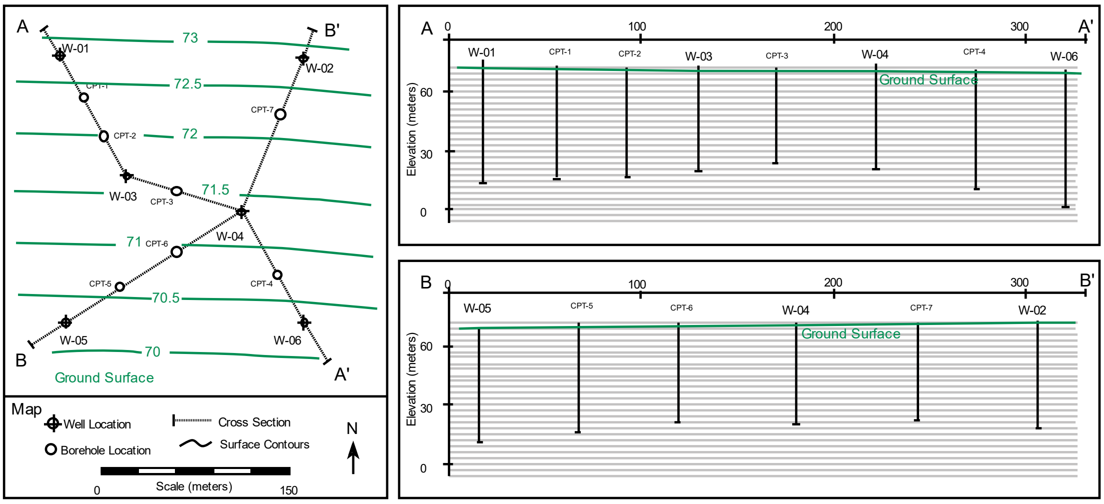


Figure 1 - The interpretation framework (Brandenburg, 2020).

4.2 Surfaces

Geologic interpretation involves dividing the subsurface into layers. Stratigraphers are interested in horizons and zones representing specific geological times, structural geologists try to identify surfaces that were originally horizontal, and geophysicists look for layers with contrasting acoustic rock properties. No matter the basis, constructing three-dimensional surfaces is an essential part of subsurface geological modeling. The most robust way to do this is to contour the data defining the surface of interest, creating structural contours: maps with lines of equal elevation defining the geologic surface of interest. Structural contour maps are analogous to topographic contour maps.

Contouring by hand (Figure 2) instead of relying on a computer algorithm has the benefit of incorporating human understanding of typical geologic characteristics, whereas software does not have the benefit of common sense in areas of sparse data. Hand-contoured maps are useful as quality control on contours generated using computer software, particularly for surfaces that are discontinuous because of faulting.

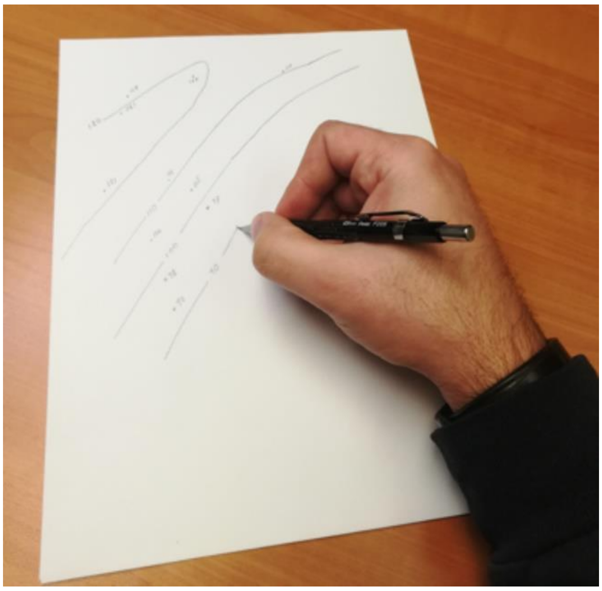


Figure 2 - Drawing structural contours by hand is a reliable method for geologic interpretation (Brandenburg, 2020).

At the Test Site, detailed lithological logs were generated for each borehole using a combination of samples collected during drilling and those collected by borehole sensing devices (Figure 3). Here, lithological logs were generated using a Cone Penetrometer Test (CPT): a method of directly sensing changes in the mechanical properties of the unconsolidated materials during drilling. CPT is commonly employed for environmental investigations and has the benefit of producing logs in discrete intervals rather than a continuous curve. For the Test Site, the discrete lithological logs differentiate between bedrock and six classes of clay, silt, sand, and gravel.

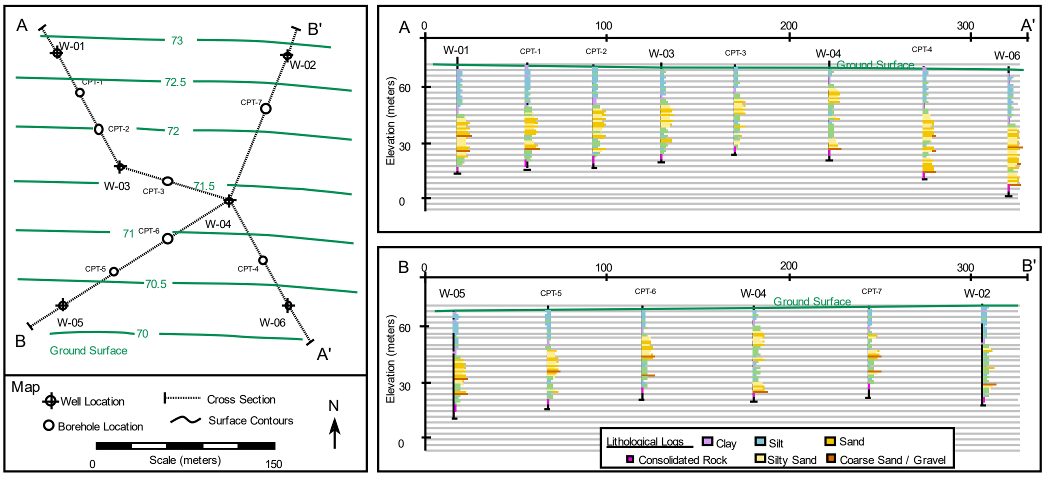


Figure 3 - Discrete lithological logs at the Test Site. The surface contours show the elevation of the ground surface above sea level (Brandenburg, 2020).

Analysis of the logs reveals fining upward sediments thinning over a bedrock high. The key surfaces identified are the top of the bedrock, and a laterally continuous clay separating the coarser strata from shallower silts and clays. Based on slightly artesian conditions observed when installing the monitoring wells, the clay layer behaves as a leaky aquitard. This is mapped as stratigraphic horizon H01 as shown in

Figure 4. Based on familiarity with similar sites in the region, the horizon is mapped as a roughly symmetrical anticline.

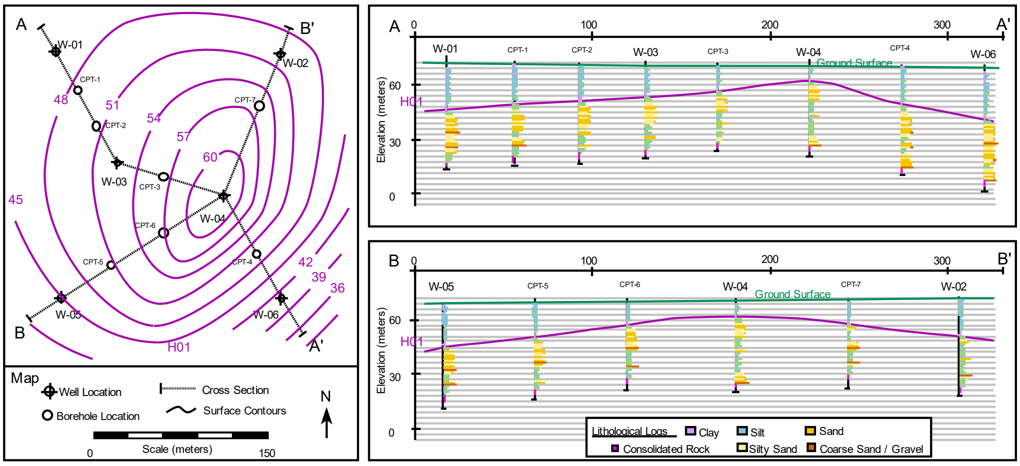


Figure 4 - Stratigraphic Horizon H01. The surface contours show the elevation of stratigraphic horizon H01 above sea level (Brandenburg, 2020).

The bedrock in this location is known to be faulted by northeast-southwest trending normal faults. The scarp was identified by a coarse-grained unit present at the base of borehole W-04 but not observed in other wells. The stratigraphic interval thickness between H01 and Bedrock is thicker in wells W-04, CPT--7 and W-02 compared to the thickness in wells CPT-6, CPT-5 and W-05. This indicates that the fault is a growth fault that most likely does not reach the H01 level. This results in the need for an offset in the bedrock surface in the contour map shown in Figure 5.

This type of small buried fault scarp is common, particularly in tectonically active areas such as the Western United States. Interpretation of faults in boreholes is another rich topic beyond the scope of this book. At the Test Site, the fault is important in that the sandy section is thicker and coarser on the downthrown side of the fault. If this feature were important to the project (e.g., if there was DNAPL contamination), geophysical methods that are sensitive to the depth of the sediment/bedrock interface could be employed.

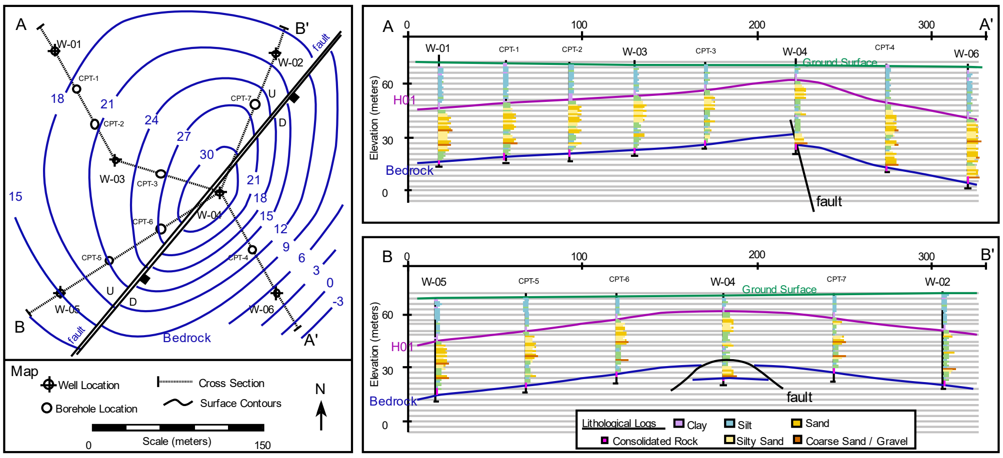


Figure 5 - The structured surface defining the top of bedrock. The surface contours show the elevation of the top of bedrock above sea level. Contours are discontinuous across the fault (Brandenburg, 2020, gw-project.org)

In the petroleum industry, static models are focused on the portion of the reservoir with mobile fluids. In this Test Site example, the section of interest is the coarse strata between the top of bedrock and H01. In oil and gas appraisal, the volume of rock bound between those surfaces would be referred to as the reservoir. Here, it is the aquifer. In some groundwater projects the nature of the fine-grained material is important in order to characterize their ability to store or release water, or their chemistry and potential for transferring chemical constituents via diffusion.

4.3 Gridding

Next, the surfaces defined along the cross-sections are extended using an interpolation technique (referred to as gridding) in order to define a two-dimensional plan view of their elevation. This provides an elevation for each surface of interest at regular grid intervals across the entire site and is needed for three-dimensional simulations. The simplest grid-construction method is to use point observations like the elevation of a stratum in particular wells as direct input to gridding algorithms, which can be done in commercial programs such as EVS↗ or Surfer↗. These programs are primarily intended for data visualization but can be also be used to prepare gridded surfaces for models.

The quality of input data is very important to this process. The ideal dataset contains points that are evenly spaced, cover the entire area that will be gridded, and have been reviewed for inconsistencies and validated. Given such a dataset, most algorithms will produce the same gridded surface. Use of sparse, irregularly spaced and internally inconsistent data is a major source of error in geologic modeling. The output of different gridding algorithms can vary drastically in the response to inconsistent data and data outliers. Some common gridding artifacts are bull's eyes around single data points and surfaces that extend significantly beyond the limits of the original data (See **Box 1** for examples⤵).

In situations with sparse or irregular data, a systematic and ideally geology-based method is required to guide the gridding algorithm in this “white space” between observations. Software available for this type of 3D geologic modeling, for example Visual MODFLOW Flex↗ and RockWorks↗. For the Test Site, the relatively simple method of digitizing hand-drawn contours to create additional data points for the gridding algorithm is used since it requires no special software (Figure 6).

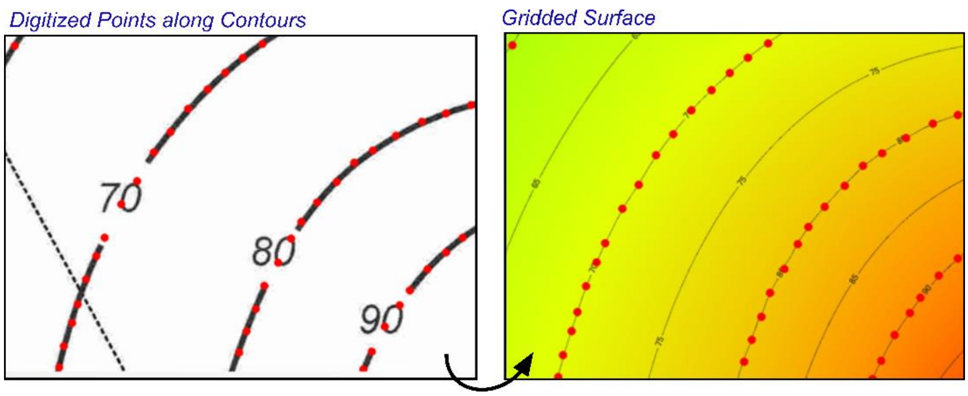


Figure 6 - Gridding algorithms need guidance in areas with sparse data. Here, hand-drawn contours are digitized to provide data to the gridding algorithm (Brandenburg, 2020).

In the Test Site model, the hand contoured data were digitized then gridded with 50 by 50 grid node discretization (grid cells are approximately 15 meters by 15 meters). This ‘50x50 grid’ is used for calculations throughout the rest of the book.

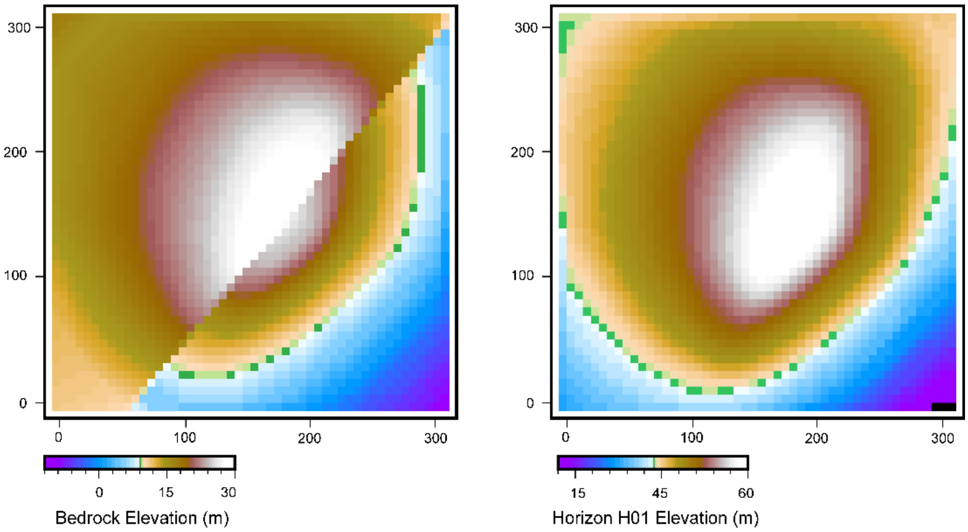


Figure 7 - Gridded surfaces for top bedrock (left) and H01 (right). Each square is an interpolated value of the elevation of the surface with its magnitude indicated by the color of the square. Plotted with the Open-Source Generic Mapping Tools (GMT↗) (Brandenburg, 2020).

5 Calculating Properties

Once the three-dimensional framework is defined and gridded, the next step is to populate the grid with the hydraulic property values needed for the simulation

5.1 Gross Thickness

The simplest property is the thickness of the reservoir or aquifer, which is the vertical distance between the bounding surfaces (Figure 8).

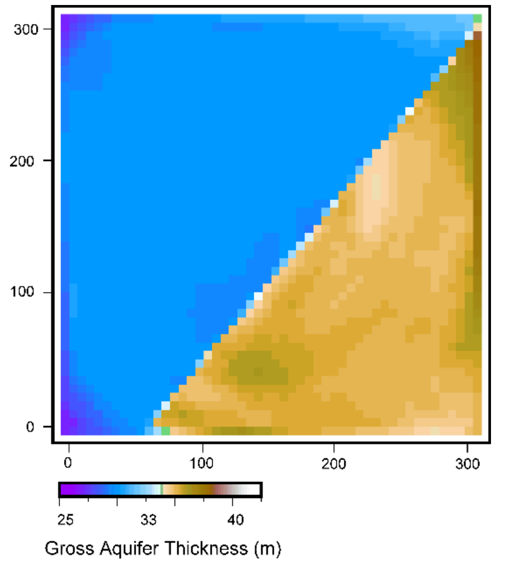


Figure 8 - The gridded aquifer thickness is the difference between the grid for HO1 and the bedrock surface (Brandenburg, 2020).

For dipping or folded strata, it may be necessary to apply a trigonometric dip correction (Figure 9). In the Test Site example, structural deformation is relatively minor, so no dip correction is applied.

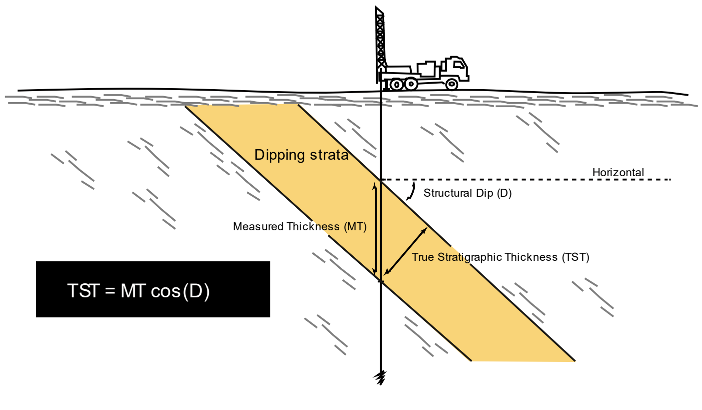


Figure 9 - Calculating true stratigraphic thickness from borehole measurement of a dipping stratum (Brandenburg, 2020).

5.2 Net Thickness

Clays and related rocks such as shale have volumetrically large but disconnected porosity and represent a volume of the aquifer that is not involved in active flow, which is important in evaluating groundwater contamination sites (Payne et al., 2008). The "flowing" portion of the reservoir or aquifer is identified as "net section". To determine this, a cutoff-value of coarseness is selected, and the geologic logs are "blocked" into net (coarse sediments) and non-net (fine sediments) zones. The thickness of the net section is tallied for each log, and then used to create contours of net thickness as shown in Figure 10. In this case, the map is an isopach where isocontours represent lines of constant thickness rather than constant elevation.

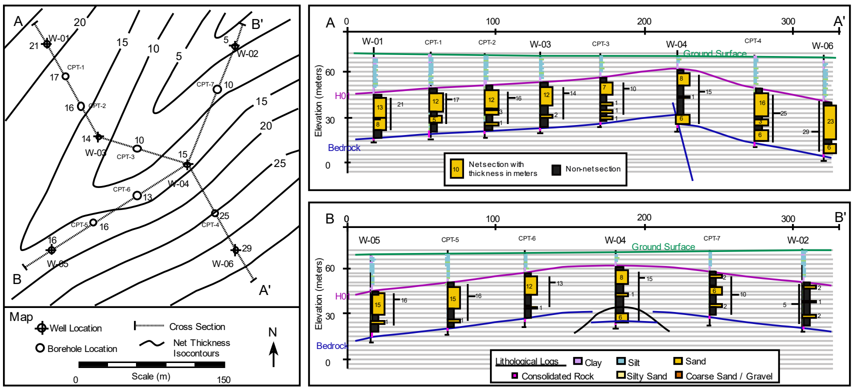


Figure 10 - Quantifying Net Thickness with blocked logs and an isopach map (Brandenburg, 2020).

The thickness contours are then gridded using the same process as the horizons in the previous steps (Figure 11).

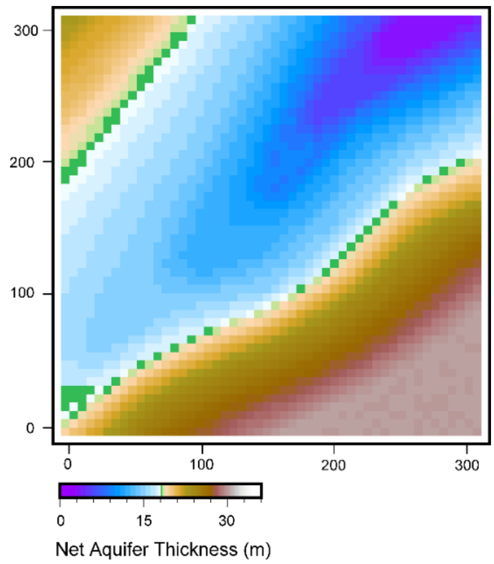


Figure 11 - Gridded Net Thickness Map (Brandenburg, 2020, gw-project.org)

5.3 Net to Gross Ratio

Once data for net and gross thickness have been mapped and gridded, it is straightforward to take the ratio of the two. Net thickness divided by total thickness is the net to gross thickness ratio, a value between 0 and 1 that is usually just referred to as net to gross (Figure 12). Regardless of sedimentary facies, high net to gross layers tend to prove both permeable and hydraulically well connected. While low net to gross layers can be permeable at individual wells, they are much more likely to be broken into disconnected compartments.

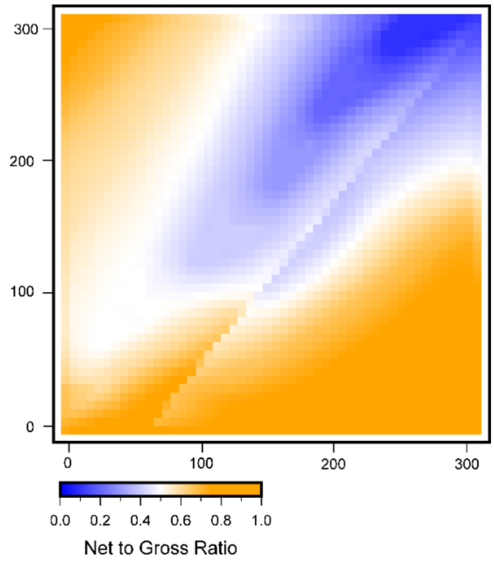


Figure 12 - Gridded Net to Gross Ratio (Brandenburg, 2020).

5.4 Properties

In oil and gas reservoir appraisal, the net to gross thickness ratio in clastic reservoirs has been long known to correlate reliably with several bulk reservoir properties. Porosity and permeability are often mapped directly from the net to gross value using interpolation functions unique to a particular oil field. At the Test Site, porosity and hydraulic conductivity are estimated based on the correlation between net to gross ratio and the porosity and hydraulic conductivity measurements made in the permanent monitoring wells as shown in Figure 13.

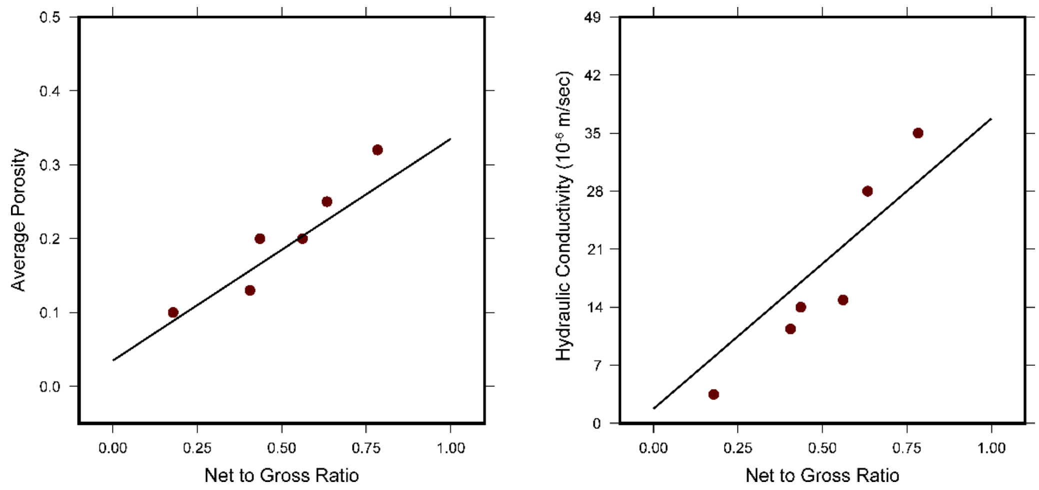


Figure 13 - Relationship between net to gross ratio of each well and the porosity and hydraulic conductivity measurements made in the well (Brandenburg, 2020).

The equations for the lines in Figure 13 are (Equations 1 and 2):

$$Porosity = \phi = 0.3\left[\frac{N}{G}\right] + 0.035 \tag{1}$$

$$\boldsymbol{Hydraulic\ Conductivity = K = (35x10^{-6})\left[\frac{N}{G}\right] + (1.8x10^{-6})} \tag{2}$$

Once these aquifer specific relationships have been established, they can be calculated for each grid location given its net to gross value to create aquifer properties for each cell of the 50x50 grid (Figure 14).

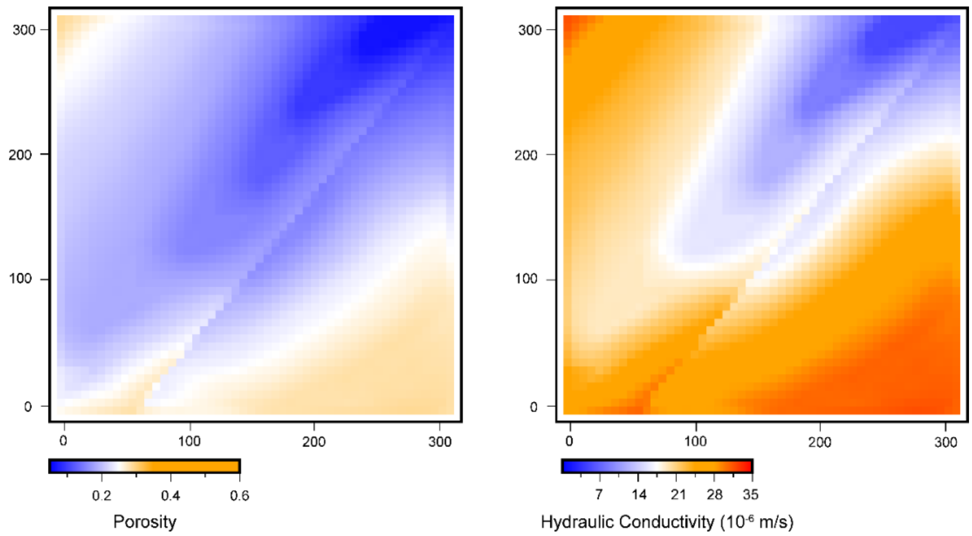


Figure 14 - Gridded porosity and hydraulic conductivity calculated from Equations 1 and 2 (Brandenburg, 2020)

6 The Model

The model shown in Figure 15 was assembled using Visual Modflow FLEX, with the grid populated using the porosity and hydraulic conductivity relationships from the previous section.

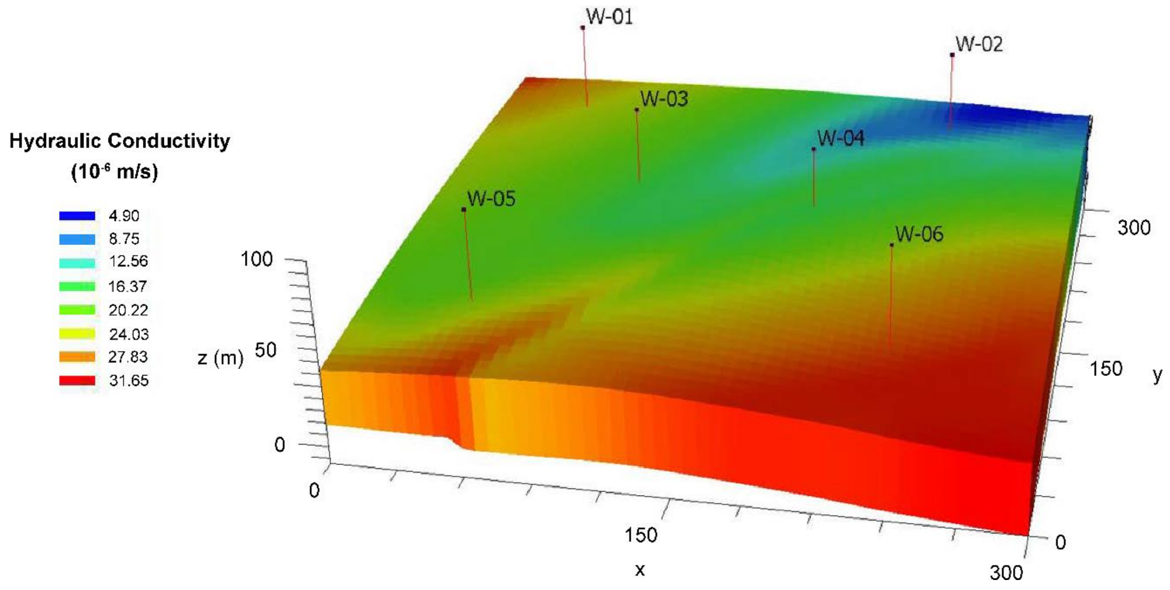


Figure 15 - Hydraulic Conductivity mapped to the three-dimensional model grid in Visual MODFLOW FLEX (Brandenburg, 2020).

At this point, the model is ready to be used for dynamic simulations. However, this model is presented to illustrate principles of subsurface delineation from borehole data. It represents the site as a single layer, while groundwater models typically require multiple layers to represent groundwater systems with multiple aquifers, engineered features within a groundwater system, and/or complex geologic heterogeneity, especially when contaminant transport or remediation is simulated.

For a multi-layer model, stratigraphic horizons can be modeled using the same methods described in this book. Geostatistical methods may also be applied; for example, most groundwater modeling pre-processing software allow properties such as hydraulic conductivity to be interpolated between observed values using a geostatistical algorithm such as Kriging.

7 Building a Static Model from Facies Mapping

A method frequently used for capturing heterogeneity in petroleum static models is facies mapping. Geological facies are assemblages of rocks, sediments or soils with a common origin and geologic history, which in this context would lead to similar hydrological behavior. For example, in a fluvial system, floodplain sediments would tend to have abundant fine-grained, layered muds, creating low hydraulic conductivity, and ratio of vertical to horizontal connectivity much less than one. Conversely, a gravel point bar deposit would have a high hydraulic conductivity with the ratio of vertical to hydraulic conductivity closer to unity. In facies mapping, each grid cell is assigned a facies code, which is then "mapped" to a corresponding set of hydraulic parameters (Figure 16).

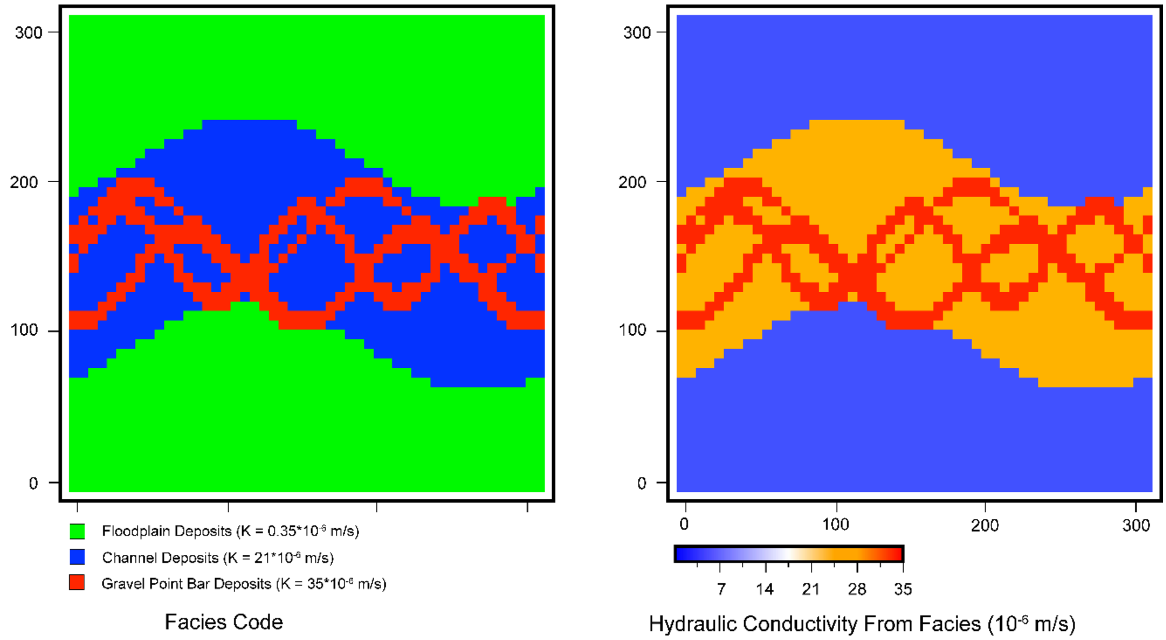


Figure 16 - Hydraulic conductivity properties from facies mapping (Brandenburg, 2020).

Of course, the facies are only known at the location of the boreholes; the rest must be assigned by some process. In the simplest scenario this is assigned based on the intuition of the modeler. However, many different but equally valid facies maps could be developed. This is the basis for more advanced geostatistical models that simultaneously honor both statistical constraints and geologic principles. Some of these models are very complex and represent the types of heterogeneity observed in carefully measured rock outcroppings and other geological studies at a much finer scale that the grid resolution of the flow model. Using this as the basis for a flow model requires a quantitative upscaling technique to make sure that the fine-scale flow properties are retained in the coarser grid.

8 Building a Static Model from Upscaled Properties

A more direct but also labor-intensive methodology is to populate the model using hydraulic properties "upscaled" from the finest scale data available. If cores are collected from a borehole, undisturbed soil or rock samples can be sent to a laboratory for porosity and hydraulic conductivity tests. This allows for correlation between lithology and hydraulic properties on the scale of inches. A representative volume is then built with a layering scheme following the major lithology types in the core. Each layer is assigned a "blended" hydraulic conductivity that represents a statistical average of laboratory measurements for that lithology. These layers are then translated to a bulk vertical (Kv) and horizontal (Kh) hydraulic conductivity (Figure 17).

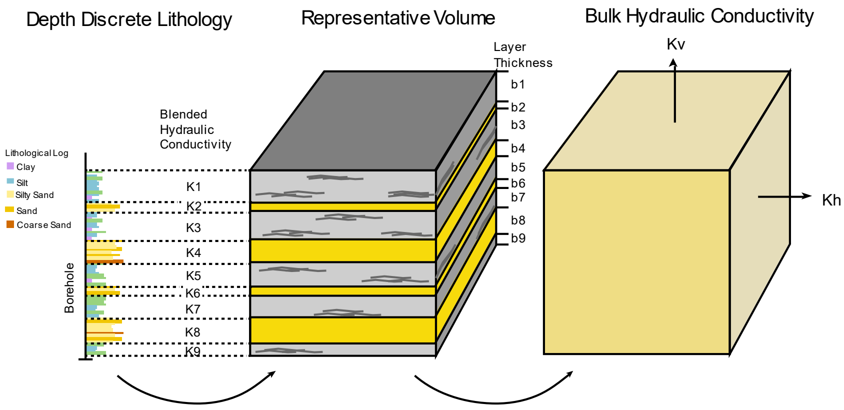


Figure 17 - Upscaling from depth discrete to bulk hydraulic conductivity (Brandenburg, 2020).

Bulk horizontal hydraulic conductivity is calculated as the arithmetic mean of the blended layers, as shown in Equation 3 for the example in Figure 17.

$$\boldsymbol{Kh} = \frac{\boldsymbol{K_1 b_1 + K_2 b_2 + K_3 b_3 + K_4 b_4 + K_5 b_5 + K_6 b_6 + K_7 b_7 + K_8 b_8 + K_9 b_9}}{\boldsymbol{b_1 + b_2 + b_3 + b_4 + b_5 + b_6 + b_7 + b_8 + b_9}} \tag{3}$$

Bulk porosity is also calculated was an arithmetic mean. Bulk vertical hydraulic conductivity is calculated as the harmonic mean of the blended layers, as shown in Equation 4 for the example in Figure 17.

$$\boldsymbol{Kv} = \frac{\boldsymbol{b_1 + b_2 + b_3 + b_4 + b_5 + b_6 + b_7 + b_8 + b_9}}{\boldsymbol{\frac{b_1}{K_1} + \frac{b_2}{K_2} + \frac{b_3}{K_3} + \frac{b_4}{K_4} + \frac{b_5}{K_5} + \frac{b_6}{K_6} + \frac{b_7}{K_7} + \frac{b_8}{K_8} + \frac{b_9}{K_9}}} \tag{4}$$

In general, the harmonic mean is representative of K for layers perpendicular to the flow direction, while the arithmetic mean represents K for layers parallel to flow. While accurate in a volume immediately surrounding the borehole, some systematic method is still required to extend these results to the rest of the model volume. In practice, this is often accomplished by combining upscaling with stochastic modeling methods.

9 Building a Static Model from Lithologic Data

When sufficient geologic data are available for defining a groundwater modeling framework, modeling software such as RockWorks↗ can be used to create a grid of lithologic types throughout the model domain, with hydraulic properties assigned to each lithologic type (Figure 18). An animated view of the model is presented in this video↗. The 35 second (~80Mb) animation rotates the basin in three-dimensional space while showing: the bedrock surface; the lithologic logs used to determine the lithology distribution; fence diagrams along a few cross sections; and the final solid model sequentially sliced from west to east and back, then from south to north and back. Fine-grained materials are displayed as purple, medium-grained as yellow, and coarse-grained as orange with faults as red.

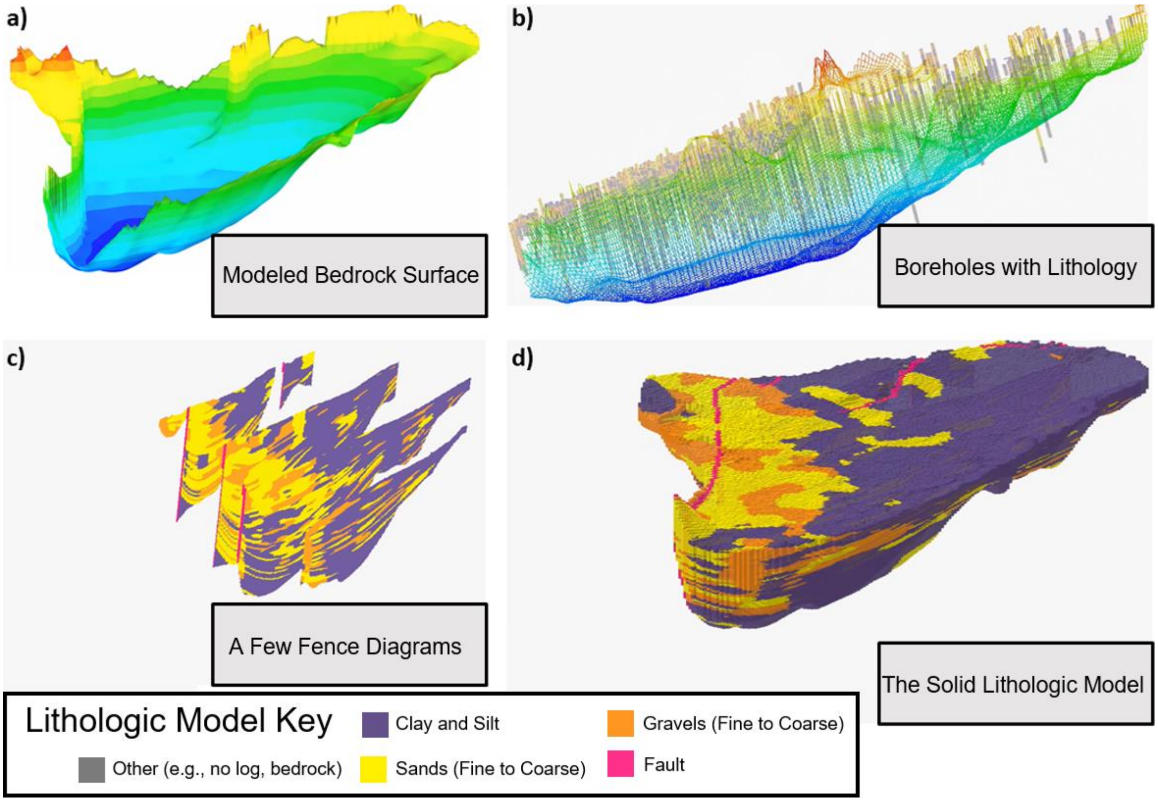


Figure 18 - Lithologic model starting with a) definition of the bedrock surface; definition of lithologic types in each borehole; c) a few fence diagrams after lithologic types are interpolated and extrapolated between wells; and d) the full solid lithologic model. Images provided by RockWare (2020).

10 Summary

Subsurface modeling concepts in this book were presented in the context of the static to dynamic model workflow. Every groundwater project is unique, and such workflows should be viewed more as a recommended organizational structure rather than a strict procedure. The typical sparsity of data constraints at the site level makes the initial conceptualization of structural and stratigraphic models the critical first step in the process.

Workflow approaches have the benefit of providing a process to make sure that edits to assumptions and data constraints propagate though all levels of the completed project.

While some of the techniques discussed apply only to clastic aquifers, the method of constructing a 3D model framework from maps, cross sections, and contoured surfaces is universally applicable. All of the more advanced statistical and lithological modeling discussed still rely on a robust 3D framework. Sketching 3D frameworks out on pencil and paper or whiteboard as a team are also an excellent way to build consensus, define assumptions and facilitate communication. Using this as a starting point for modeling projects is a best practice.

11 References

Brandenburg, J.P., 2020, Original figures.

Payne, F., J. Quinnan, and S. Potter, 2008, Remediation Hydraulics, 1st Edition. Chemical Rubber Company (CRC) Press.

RockWare, 2020, https://ww.rockware.com/product/rockworks/↗.

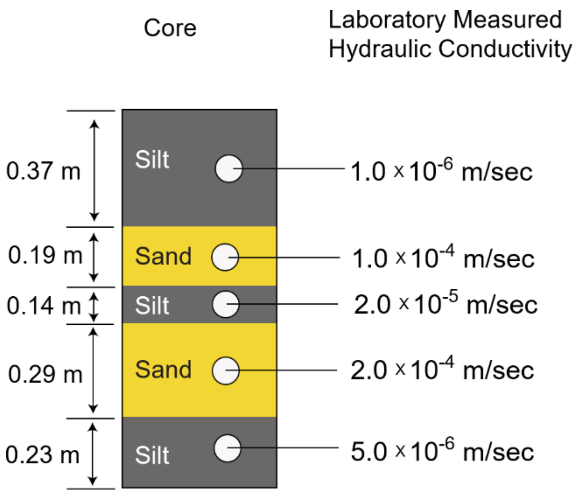
Schultz, M., R. Cramer, C. Plank, H. Levine, K. Ehman, 2017, Best practices for environmental site management: A practical guide for applying environmental sequence stratigraphy to improve conceptual site models. Technical Report. https://cfpub.epa.gov/si/si_public_file_download.cfm?p_download_id=536250&Lab=NRMRL↗.

Shepherd, M., 2009, Oil field production geology, AAPG Memoir 91, The American Association of Petroleum Geologists, Tulsa, Oklahoma, 350p.

12 Exercises

One method to analyze soil and rock cores collected during drilling is to measure hydraulic properties of small centimeter-sized samples removed from the larger core (“core plugs”) in a laboratory. Before the results can be used for flow simulations, calculations of bulk properties are required.

Consider the following core collected from a deposit of layered silt and sand. The core is 1.22 meters long, and oriented vertically. Hydraulic conductivity was calculated for five core plugs:



Exercise 1

If only the flow of groundwater through the sand is significant, what is the net/gross ratio of this core?

Click here for solution to exercise 1

Exercise 2

What are the calculated bulk vertical and horizontal hydraulic conductivities of the representative volume?

Click here for solution to exercise 2

Exercise 3

What else would you need before using the calculated bulk hydraulic properties for a flow model?

Click here for solution to exercise 3

Box 1 Gridding Sparse Data

With data from a sufficient number of boreholes, all gridding algorithms should reproduce the same geologic surface. With sparse data, the surfaces will diverge from one another. For the Test Site, gridding of the H01 surface using only the elevation data measured in the 14 boreholes is shown using a few different methods in **Figure Box 1-1**.

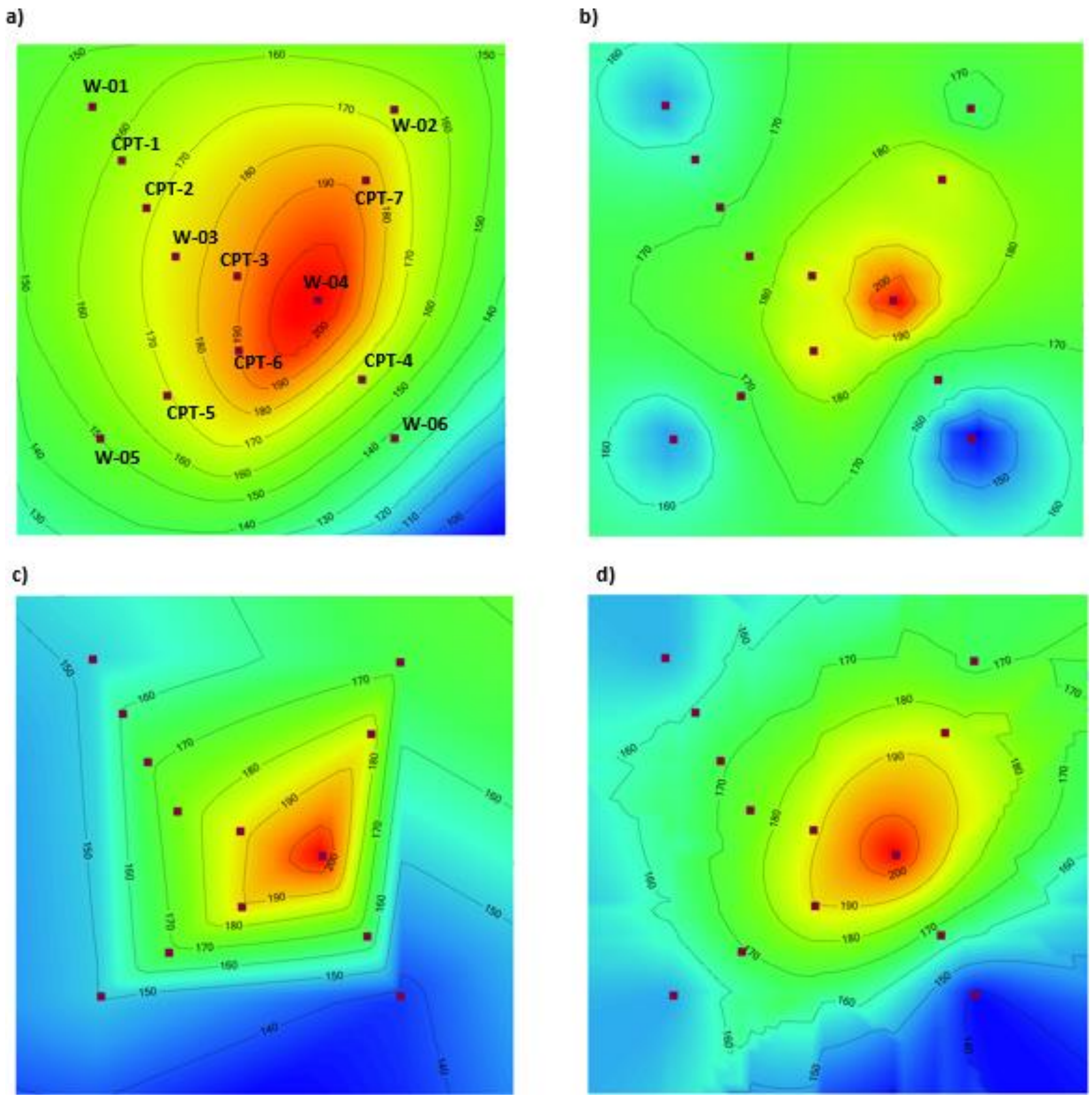


Figure Box 1-1 - Gridding of the H01 surface using only the elevation data measured in the 14 boreholes using: a) hand-drawn structural contours representing geologic “reality”; b) inverse distance algorithm; c) natural neighbors algorithm; and, d) Kriging algorithm. (Brandenburg, 2020, gw-project.org)

These images were created with the gridding algorithms available in Visual MODFLOW FLEX (Waterloo Hydrogeologic, 2020) using mainly default parameters. With experience, the gridding parameters can be adjusted to create a surface closer to what is expected for H01. This is particularly true for Kriging, which is designed for irregular geologic datasets. However, no matter the choice of algorithm, some prior concept of the geology is required.

Performance of gridding algorithms is always poorest near the periphery of the grid. The algorithms perform *interpolation* inside of the area delineated by the datapoints, and *extrapolation* outside. Extrapolation is inherently more uncertain, which can result in gridding artifacts when the boundary is far from the data points.

Return to where text links to Box 1 ↥

13 Exercise Solutions

Exercise 1 – Solution

If only the flow of groundwater through the sand is significant, what is the net/gross ratio of this core?

$$\boldsymbol{Net/Gross} = \frac{\mathbf{0.19+0.29}}{\mathbf{0.37+0.19+0.14+0.29+0.23}} = \mathbf{0.39}$$

Return to Exercise 1↥

Exercise 2 – Solution

What are the calculated bulk vertical and horizontal hydraulic conductivities of the representative volume?

$$\boldsymbol{Kv} = \frac{\mathbf{0.37+0.19+0.14+0.29+0.23}}{\frac{\mathbf{0.37}}{\mathbf{1.0x10^{-6}}}+\frac{\mathbf{0.19}}{\mathbf{1.0x10^{-4}}}+\frac{\mathbf{0.14}}{\mathbf{2.0x10^{-5}}}+\frac{\mathbf{0.29}}{\mathbf{2.0x10^{-4}}}+\frac{\mathbf{0.23}}{\mathbf{5.0x10^{-6}}}}$$

Vertical bulk hydraulic conductivity = $\boldsymbol{Kv} = \mathbf{2.9x10^{-6}}\ \frac{\boldsymbol{m}}{\boldsymbol{s}}$

$$\boldsymbol{Kh} = \frac{(\mathbf{1.0x10^{-6}} * \mathbf{0.37}) + (\mathbf{1.0x10^{-4}} * \mathbf{0.19}) + (\mathbf{2.0x10^{-5}} * \mathbf{0.14}) + (\mathbf{2.0x10^{-4}} * \mathbf{0.29}) + (\mathbf{5.0x10^{-6}} * \mathbf{0.23})}{\mathbf{0.37+0.19+0.14+0.29+0.23}}$$

Horizontal bulk hydraulic conductivity = $\boldsymbol{Kh} = \mathbf{6.7x10^{-5}}\ \frac{\boldsymbol{m}}{\boldsymbol{s}}$

Return to Exercise 2↥

Exercise 3 – Solution

What else would you need before using the calculated bulk hydraulic properties for a flow model?

You would need to know how this core fits within the geological framework of the model. Some key questions to ask: What is the scale of the model compared to the scale of the core? This core would be reasonably representative of flow units that are a few meters thick, but not for units that are tens of meters thick. Are the stratigraphic horizons horizontal, or do they have a measurable dip? If so, it may be necessary to apply a dip correction, as in Section 5. Keep in mind that the geology likely varies as much horizontally as it does vertically, so additional cores would be necessary to apply this methodology rigorously.

Return to Exercise 3↥

14 About the Author

Dr. JP Brandenburg is a professional geologist at Haley & Aldrich where he performs groundwater modeling for a variety of environmental, mining and water resource applications. He began his numerical modeling career in geodynamics, studying viscous convection in Earth's mantle at the University of Michigan. He then joined the research organization at Royal Dutch Shell, developing methods for modeling complex subsurface structural geology in hydrocarbon reservoirs. After several years of deploying these techniques in Shell's exploration and production organization, Dr. Brandenburg changed focus to the environmental industry. In addition to applied modeling, he continues to build on cross disciplinary experience to develop new methods for capturing subsurface geological heterogeneity. Dr. Brandenburg has a number of publications in geodynamics, petroleum geology, structural geology, and numerical modeling.

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Modifications to Original Release

General changes:

Bold font in equations was removed except for the final answer in the exercise solutions.

External links in blue font within the body of the book were changed to black font.

The external link symbol was added after links where it was missing.

The internal link symbol was added after links where it was missing.

False bookmarks were removed from the navigation pane.

Specific changes:

page iii, Added citation information and the book DOI.

page 9, “20 by 20” was changed to “50 by 50”

page 9, “20x20” was changed to “50x50”

page 9, A hyphen was added in the caption of Figure 7 between the words: “Open” and “Source”.

page 13, “20x20” was changed to “50x50”

page 16, Denominator of equation 4 was corrected to change b_8/K_5 to b_8/K_8 and to include the additional term b_9/K_9

page 18, An erroneous line break was removed from the last reference.