Quantifying Uncertainty in Subsurface Systems



Céline Scheidt, Lewis Li, and Jef Caers *Editors*





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PREFACE

"I think that when we know that we actually do live in uncertainty, then we ought to admit it; it is of great value to realize that we do not know the answers to different questions. This attitude of mind – this attitude of uncertainty – is vital to the scientist, and it is this attitude of mind which the student must first acquire"

Richard P. Feynman, Noble Laureate in Physics, 1965

This book offers five substantial case studies on decision making under uncertainty for subsurface systems. The strategies and workflows designed for these case studies are based on a Bayesian philosophy, tuned specifically to the particularities of the subsurface realm. Models are large and complex; data are heterogeneous in nature; decisions need to address conflicting objectives; the subsurface medium is created by geological processes that are not always well understood; and expertise of a large variety of scientific and engineering disciplines need to be synthesized.

There is no doubt that we live in an uncertain time. With growing population, resources such as energy, materials, water, and food will become increasingly critical in their exploitation. The subsurface offers many such resources, important to the survival of humankind. Drinking water from groundwater systems is gaining in importance, as aquifers are natural purifiers and can store large volumes. However, the groundwater system is fragile, subject to contamination from agriculture practices and industries. Before renewables become the dominant energy sources, oil and gas will remain a significant resource in the next few decades. Geothermal energy both deep (power) and shallow (heating) can contribute substantially to alleviating reliance on fossil fuels. Mining minerals used for batteries will aid in addressing intermittency of certain renewables, but mining practices will need to address environmental concerns.

Companies and governmental entities involved in the extraction of these resources face considerable financial risk because of the difficulty in accessing the poorly understood subsurface and the cost of engineering facilities. Decisions regarding exploration methods, drilling, extraction methods, and data-gathering campaigns often need to balance conflicting objectives: resource versus environmental impact, risk versus return. This can be truly addressed only if one accepts uncertainty as integral part of the decision game. A decision based on a deterministic answer when uncertainty is prevailing is simply a poor decision, regardless of the outcome. Decisions and uncertainty are part of one puzzle; one does not come before the other.

Uncertainty on key decision variables such as volumes, rates of extraction, time of extraction, spatiotemporal variation on fluid movements needs to be quantified. Uncertainty quantification, in this book shortened to UQ, requires a complex balancing of several fields of expertise such as geological sciences, geophysics, data science, computer science, and decision analysis. We gladly admit that we do not have a single best solution to UQ. The aim of this book is to provide the reader with a principled approach, meaning a set of actions motivated by a mathematical philosophy based on axioms, definitions, and algorithms that are well understood, repeatable, and reproducible, as well as a software to reproduce the results of this book. We consider uncertainty not simply to be some posterior analysis but a synthesized discipline steeped in scientific ideas that are still evolving. Ten chapters provide insight into our way of thinking on UQ.

Chapter 1 introduces the five case studies: an oil reservoir in Libya, a groundwater system in Denmark, a geothermal source for heating buildings in Belgium, a contaminated aquifer system in Colorado, and an unconventional hydrocarbon resource in Texas. In each case study, we introduce the formulation of the decision problem, the types of data used, and the complexity of the modeling problem. Common to all these cases is that the decision problem involves simple questions: Where do we drill? How much is there? How do we extract? What data to gather? The models involved on the other hand are complex and high dimensional, the forward simulators time-consuming. The case studies set the stage.

Chapter 2 introduces the reader to some basic notions in decision analysis. Decision analysis is a science, with its own axioms, definitions, and heuristics. Properly formulating the decision problem, defining the key decision variables, the data used to quantify these, and the objectives of the decision maker are integral to such decision analysis. Value of information is introduced as a formal framework to assess the value of data before acquiring it.

Chapter 3 provides an overview of the various data science methods that are relevant to UQ problems in the subsurface. Representing the subsurface requires a highdimensional model parametrization. To make UQ problems manageable, some form of dimension reduction is needed. In addition, we focus on several methods of regression such as Gaussian process regression and CART (classification and regression trees) that are useful for statistical learning and development of statistical proxy models. Monte Carlo is covered extensively as this is instrumental to UQ. Methods such as importance sampling and sequential importance resampling are discussed. Lastly, we present the extension of Monte Carlo to Markov chain Monte Carlo and bootstrap; both are methods to address uncertainty and confidence.

Chapter 4 is dedicated to sensitivity analysis (SA). Although SA could be part of Chapter 3, because of its significance to UQ, we dedicate a single chapter to it. Our emphasis will be on global SA and more specifically Monte Carlo-based SA since this family of methods (Sobol', regionalized sensitivity analysis, CART) provides key insight into understanding what model variables most impact data and prediction variables.

Chapter 5 introduces the philosophy behind Bayesian methods: Bayesianism. We provide a historical context to why Bayes has become one of the leading paradigms to UQ, having evolved from other paradigms such as induction, deduction, and falsification. The most important contribution of Thomas Bayes is the notion of the prior distribution. This notion is critical to UQ in the subsurface, simply because of the poorly understood geological medium that drives uncertainty. The chapter, therefore, ends with a discussion on the nature of prior distributions in the geosciences, how one can think about them and how they can be established from physical, rather than statistical principles.

Chapter 6 then extends on Chapter 5 by discussion on the role of prior distribution in inverse problems. We provide a brief overview of both deterministic and stochastic inversion. The emphasis lies on how quantification of geological heterogeneity (e.g., using geostatistics) can be used as prior models to solve inverse problems, within a Bayesian framework.

Chapter 7 is perhaps the most novel technical contribution of this book. This chapter covers a collection of methods termed Bayesian evidential learning (BEL). Previous chapters indicated that one of the major challenges in UQ is model realism (geological) as well as deal with large computing times in forward models related to data and prediction responses. In this chapter, we present several methods of statistical learning, where Monte Carlo is used to generate a training set of data and prediction variables. This Monte Carlo approach requires the specification of a prior distribution on the model variables. We show how learning the multivariate distribution of data and prediction variables allows for predictions based on data without complex model inversions.

Chapter 8 presents various strategies addressing the decision problem of the various case studies introduced in Chapter 1. The aim is not to provide the best possible method but to outline choices in methods and strategies in

combination to solve real-world problems. These strategies rely on materials presented in Chapters 2–7.

Chapter 9 provides a discussion of the various software components that are necessary for the implementation of the different UQ strategies presented in the book. We discuss some of the challenges faced when using existing software packages as well as provide an overview of the companion code for this book.

Chapter 10 concludes this book by means of seven questions that formulate important challenges that when addressed may move the field of UQ forward in impactful ways.

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We hope you enjoy our work.

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The Earth Resources Challenge

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1.1. WHEN CHALLENGES BRING OPPORTUNITIES

Humanity is facing considerable challenges in the 21st century. Population is predicted to grow well into this century and saturate between 9 and 10 billion somewhere in the later part. This growth has led to climate change (see the latest IPCC reports), has impacted the environment, and has affected ecosystems locally and globally around the planet. Virtually no region exists where humans have had no footprint of some kind [Sanderson et al., 2002]; we now basically "own" the ecosystem, and we are not always a good Shepard. An increasing population will require an increasing amount of resources, such as energy, food, and water. In an ideal scenario, we would transform the current situation of unsustainable carbon-emitting energy sources, polluting agricultural practices and contaminating and over-exploiting drinking water resources, into a more sustainable and environmentally friendly future. Regardless of what is done (or not), this will not be an overnight transformation. For example, natural gas, a green-house gas (either as methane or burned into CO_2), is often called the blue energy toward a green future. But its production from shales (with vast amounts of gas and oil reserves, 7500 Tcf of gas, 400 billion barrels of oil, US Energy Information, December

³Anadarko, The Woodlands, TX, USA

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⁵Department of Energy Resources Engineering, Stanford University, Stanford, CA, USA 2014) has been questioned for its effect on the environment from gas leaks [*Howarth et al.*, 2014] and the unsolved problem of dealing with the waste water it generates. Injecting water into kilometer-deep wells has caused significant earthquakes [Whitaker, 2016], and risks to contamination of the groundwater system are considerable [*Osborn et al.*, 2011].

Challenges bring opportunities. The Earth is rich in resources, and humanity has been creative and resourceful in using the Earth to advance science and technology. Batteries offer promising energy storage devices that can be connected to intermittent energy sources such as wind and solar. Battery technology will likely develop further from a better understanding of Earth materials. The Earth provides a naturally emitting heat source that can be used for energy creation or heating of buildings. In this book, we will contribute to exploration and exploitation of geological resources. The most common of such resources are briefly described in the following:

1. *Fossil fuels* will remain an important energy source for the next several decades. Burning fossil fuels is not a sustainable practice. Hence, the focus will be on the transformation of this energy, least impacting the environment as possible. An optimal exploitation, by minimizing drilling, will require a better understanding of the risk associated with the exploration and production. Every mistake (drilling and spilling) made by an oil company has an impact on the environment, direct or indirect. Even if fossil fuels will be in the picture for a while, ideally we will develop these resources as efficient as possible, minimally impacting the environment.

2. *Heat* can be used to generate steam, drive turbines, and produce energy (high enthalpy heat systems). However, the exploitation of geothermal systems is costly and not always successful. Injecting water into

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kilometer-deep wells may end up causing earthquakes [Glanz, 2009]. Reducing this risk is essential to a successful future for geothermal energy. In a low enthalpy system, the shallow subsurface can be used as a heat exchanger, for example through groundwater, to heat buildings. The design of such systems is dependent on how efficient heat can be exchanged with groundwater that sits in a heterogeneous system, and the design is often subject to a natural gradient.

3. *Groundwater* is likely to grow as a resource for drinking water. As supply of drinking water, this resource is however in competition with food (agriculture) and energy (e.g., from shales). Additionally, the groundwater system is subject to increased stresses such as from over-pumping and contamination.

4. *Minerals resources* are exploited for a large variety of reasons. For example, the use of Cu/Fe in infrastructure, Cd/Li/Co/Ni for batteries, rare earth elements for amplifiers in fiber-optic data transmission or mobile devices, to name just a few. An increase in the demand will require the development of mining practices that have minimal effect on the environment, such as properly dealing with waste as well as avoiding groundwater contamination.

5. *Storage* of fluids such as natural gas, CO_2 , or water (aquifer storage and recovery) in the subsurface is an increasing practice. The porous subsurface medium acts as a permanent or temporary storage of resources. However, risks of contamination or loss need to be properly understood.

The geological resource challenge will require developing basic fields of science, applied science and engineering, economic decision models, as well as creating a better understanding regarding human behavioral aspects. The ultimate aim here is to "predict" what will happen, and based on such prediction what are best practices in terms of optimal exploitation, maximizing sustainability, and minimizing of impact on the environment. The following are the several areas that require research: (i) fundamental science, (ii) predictive models, (iii) data science, and (iv) economic and human behavior models.

Fundamental science. Consider, for example, the management of groundwater system. The shallow subsurface can be seen as a biogeochemical system where biological, chemical agents interact with the soils or rock within which water resides. The basic reactions of these agents may not yet be fully understood nor does the flow of water when such interactions take place. To understand this better, we will further need to develop such understanding based on laboratory experiments and first principles. Additionally, the flow in such systems depends on the spatial variability of the various rock properties. Often water resides in a sedimentary system. A better understanding of the processes that created such systems will aid in predicting such flow. However, the flow of particles in a viscous fluid, which leads to deposition and erosion

and ultimately stratigraphy, is fundamentally not well understood; hence, the basic science around this topic needs to be further developed. A common issue is that basic science is conducted in laboratories at a relatively small scale; hence, the question of upscaling to application scales remains, equally, a fundamental research challenge.

Predictive models. Fundamental science or the understanding of process alone does not result in a prediction or an improvement into what people decide in practice. Predictions require predictive models. These could be a set of partial differential equations, reactions, phase diagrams, and computer codes developed from basic understanding. In our groundwater example, we may develop codes for predictive modeling of reactive transport in porous media. Such codes require specification of initial and boundary conditions, geochemical reaction rates, biogeochemistry, porous media properties, and so on. Given one such specification, the evolution of the system can then be predicted at various space-time scales.

Data science. Predictive models alone do not make meaningful predictions in practical settings. Usually, site-specific data are gathered to aid such predictions. In the groundwater case, this may consist of geophysical data, pumping data, tracer data, geochemical analysis, and so on. The aim is often to integrate predictive models with data, generally denoted as inversion. The challenge around this inversion is that no single model predicts the data; hence, uncertainty about the future evolution of the system exists. Because of the growing complexity of the kind of data we gather and the kind of models we develop, an increased need exists in developing data scientific methods that handle such complexities fully.

Economic decision models and social behavior. The prediction of evolution of geological resource systems cannot be done without the "human context." Humans will make decision on the exploitation of geological resources and their behavior may or may not be rational. Rational decision making is part of decision science, and modeling behavior (rational or not) is part of game theory. Next to the human aspects, there is a need for global understanding of the effect of the evolution of technology on geological resources. For example, how will the continued evolution affect the economy of mineral resources? How will any policy change in terms of rights to groundwater resources change the exploitation of such resources?

In this book, we focus mostly on making predictions as input to decision models. Hence, we focus on development of data scientific tools for uncertainty quantification in geological resources systems. However, at the same time, we are mindful about the fact that we do not yet have a fundamental understanding of some of the basic science. This is important because after all UQ is about quantifying lack of understanding. We are also mindful about the fact the current predictive models only approximate any physical/chemical reality in the sense that these are based on (still) limited understanding of process. In the subsurface, this is quite prevalent. We do not know exactly how the subsurface system, consisting of solids and fluids, was created and how solids and fluids interact (together with the biological system) under imposed stresses or changes. Most of our predictive models are upscaled versions of an actual physical reality. Last, we are also mindful that our predictions are part of a larger decision model and that such decision models themselves are only approximate representation of actual human behavior.

Hence, we will not provide an exact answer to all these questions and solve the world's problems! In that sense, the book is contributing to sketching paths forward in this highly multidisciplinary science. This book is part of an evolution in the science of predictions, with a particular application to the geological resources challenge. The best way to illustrate this is with real field case studies on the above-mentioned resources, how predictive models are used, how data come into the picture, and how the decision model affects our approach to using such predictive models in actual practical cases, with actual messy data. Chapter 1 introduces these cases and thereby sets the stage.

1.2. PRODUCTION PLANNING AND DEVELOPMENT FOR AN OIL FIELD IN LIBYA

1.2.1. Reservoir Management from Discovery to Abandonment

Uncertainty quantification in petroleum systems has a long history and perhaps one of the first real-world applications of such quantification, at least for the subsurface. This is partly due to the inherent large financial risk (sometime billions of dollars) involved in decision making about exploration and production. Consider simply that the construction of a single offshore platform may cost several billion dollars and may not pay back return if uncertainty/risk is poorly understood, or if estimates are too optimistic. Uncertainty quantification is (and perhaps should be) an integral part of decision making in such systems.

Modern reservoir management aims at building complex geological models of the subsurface and running computationally demanding models of multiphase flow that simulates the combined movement of fluids in the subsurface under induced changes, such as from production by enhancing the recovery by injection of water, CO₂, polymers, or foams. In particular, for complex systems and costly operations, numerical models are used to make prediction and run numerical optimizations since simple analytical solution can only provide very rough estimates and cannot be used for individual well-planning or for assessing the worth of certain data acquisition methods.

Reservoir management is not a static task. First, the decision to use certain modeling and forecasting tools depends on what stage of the reservoir life one is dealing with, which is typically divided into (i) exploration, (ii) appraisal, (iii) early production, (iv) late production, and (v) abandonment. Additionally, several types of reservoir systems exist. Offshore reservoirs may occur in shallow to very deep water (1500-5000 ft of water column) and are found on many sedimentary margins in the world (e.g., West Africa, Gulf of Mexico, Brazil). To produce such reservoirs, and generate return on investments, wells need to be produced at a high rate (as much as 20,000 BBL/day). Often wells are clustered from a single platform. Exploration consists of shooting 2D seismic lines, from which 2D images of the subsurface are produced. A few exploration wells may be drilled to confirm a target or confirm the extent of target zone. From seismic alone it may not be certain that a sand is oil-filled or brine-filled. With interesting targets identified, 3D seismic surveys are acquired to get a better understanding of the oil/gas trap in terms of the structure, the reservoir properties, and distribution of fluids (e.g., contacts between gas/oil, oil/water). Traps are usually 1-10 km in magnitude aerially and 10-100s of feet vertically. The combination of additional exploration wells together with seismic data allows for the assessment of the amount of petroleum product (volume) available and how easy it is to recover the reservoir, and how such recovery will play out over time: the recovery factor (over time).

Because of the lack of sufficient data, any estimate of volume or recovery at the appraisal stage is subject to considerable uncertainty. For example, a reservoir volume (at surface conditions, meaning accounting for volume changes due to extraction to atmospheric conditions) is determined as

Volume = area \times thickness \times porosity \times oil saturation \times formation volume factor

(1.1)

However, this simple expression ignores the (unknown) complexity in the reservoir structure (e.g., presence of faults). Each of the above factors is subject to uncertainty. Typically, a simple Monte Carlo analysis is performed to determine uncertainty on the reservoir volume. This requires stating probability distributions for each variable, often taken as independent, and often simply guessed by the modeler. However, such analysis assumes a rather simple setting such as shown in Figure 1.1 (left). Because only few wells are drilled, the reservoir may look fairly simple from the data point of view. The combination of a limited number of wells (samples) with the low-resolution seismic (at least much lower than what can be observed in wells) may obfuscate the presence of



Figure 1.1 Idealized vs. real setting in estimating original oil in place.

complexity that affects volume, such as geological heterogeneity (the reservoir is not a homogenous sand but has a considerable non-reservoir shale portion), presence of faults not detectable on seismic, or presence of different fluid contacts as shown in Figure 1.1 (right). This requires then a careful assessment of the uncertainty of each variable involved.

While offshore reservoirs are produced from a limited set of wells (10-50), onshore systems allow for much more extensive drilling (100-1000). Next to the conventional reservoir systems (those produced in similar ways as the offshore ones and in similar geological settings), a shift has occurred to unconventional systems. Such systems usually consist of shales, which were considered previously to be "unproducible," but have become part of oil/gas production due to the advent of hydraulic fracturing (HF). Thus, starting in 2005, a massive development of unconventional shale resources throughout North America has interrupted both the domestic and the international markets. From a technical perspective, development of shale reservoirs is challenging and is subject to a substantial learning curve. To produce value, shale operators often experiment with new technologies, while also testing applicability of the best practices established in other plays. Traditional reservoir modeling methods and Monte Carlo analysis (see next) become more difficult in these cases, simply because the processes whereby rock breaks, gas/oil released and produced at the surface are much less understood and require in addition to traditional fields of reservoir science knowledge about the joint geomechanical and fluid flow processes in such systems. As a result, and because of fast development of shale plays (e.g., one company reporting drilling more than 500/year of "shale" wells), a more data centric approach to modeling and uncertainty quantification is taken. This data scientific approach relies on using production of existing wells, in combination with the production and geological parameters to directly model and forecast new wells or estimate how long a producing well will decline (hydraulic fractured wells typically start with

a peak followed by a gradual decline). In Section 1.6, we will present these types of systems. Here we limit ourselves to conventional reservoir systems.

1.2.2. Reservoir Modeling

In the presence of considerable subsurface complexity, volume or recovery factor assessment becomes impossible without explicitly modeling the various reservoir elements and all the associated uncertainties. Reservoirs requiring expensive drilling are therefore now routinely assessed by means of computer (reservoir) models, whether for volume estimate, recovery factor estimates, placement of wells, or operations of existing wells. Such models are complex, because the reservoir structure is complex. The following are the various modeling elements that need to be tackled.

1. *Reservoir charge*. No oil reservoir exists without migration of hydrocarbon "cooked" from a source rock and trapped in a sealing structure. To assess this, oil companies build basin and petroleum system models to assess the uncertainty and risk associated with finding hydrocarbons in a potential trap. This requires modeling evolution of the sedimentary basins, the source rock, burial history, heat flow, and timing of kerogen migration, all of which are subject to considerable uncertainty.

2. *Reservoir structure*, consisting of faults and layers. These are determined from wells and seismic, and these may be very uncertain in cases with complex faulting (cases are known to contain up to 1000 faults), or due to difficult and subjective interpretation from seismic. In addition, the seismic image itself (the data on which interpretation are done) is uncertain. Structures are usually modeled as surfaces (2D elements). Their modeling requires accounting of tectonic history, informing the age relationships between faults, and several rules of interaction between the structural elements (see Chapter 6).

3. *The reservoir petrophysical properties*. The most important are porosity (volume) and permeability (flow). However, because of the requirement to invert and model

seismic data (3D or 4D), other properties and their spatial distribution are required such as lithology, velocity (p-wave, s-wave), impedance, density, compressibility, Young's modulus, Poisson coefficient, and so on. First, the spatial distribution of these properties depends on the kind of depositional system present (e.g., fluvial, deltaic), which may itself be uncertain, with few wells drilled. The depositional system will control the spatial distribution of lithologies/facies (e.g., sand, shale, dolomite), which in turn controls the distribution of petrophysical properties, as different lithologies display different petrophysical characteristics. In addition, all (or most) petrophysical properties are (co)-related, simply because of the physical laws quantifying them. Rock physics is a field of science that aims to understand these relationships, based on laboratory experiments, and then apply them to understand the observed seismic signals in terms of rock and fluid properties. These relationships are uncertain because (i) the scale of laboratory experiments and ideal conditions are different from reservoir conditions and (ii) the amount of reservoir (core) samples that can be obtained to verify these relationships are limited. This has led to the development of the field of statistical rock physics [Avseth et al., 2005; Mavko et al., 2009].

4. Reservoir fluid properties. A reservoir usually contains three types of fluids: gas, oil, and brine (water), usually layered in that order because of density difference. The (initial) spatial distribution of these fluids may, however, not be homogeneous depending on temperature, pressure, geological heterogeneity, and migration history (oil matures from a source rock, traveling toward a trap). Reservoir production will initially lead to a pressure decline (primary production), then to injection of other fluids (e.g., water, gas, polymers, foams) into the reservoir. Hence, to understand all these processes, one needs to understand the interaction and movement of these various fluids under changing pressure, volume, and temperature conditions. This requires knowing the various thermodynamic properties of complex hydrocarbon chains and their phase changes. These are typically referred to as the PVT (pressure-volume-temperature) properties. The following are some basic properties involved that are crucial (to name just a few):

• Formation volume factor: The ratio of a phase volume (water, oil, gas) at reservoir conditions, relative to the volume of a surface phase (water, oil, or gas).

• Solution gas-oil ratio: The amount of surface gas that can be dissolved in a stock tank oil when brought to a specific pressure and temperature.

• API specific gravity: A common measure of oil specific gravity.

• Bubble-point pressure: The pressure when gas bubbles dissolve from the oil phase.

In a reservoir system, several fluids move jointly through the porous systems (multiphase flow). A common way to represent this is through relative permeability and capillary functions. These functions determine how one fluid moves under given saturation of another fluid. However, they in turn depend on the nature of the rock (the lithology) and the pore fabric system, which is uncertain, both in characteristics (which mineral assemblages occur) and in spatial distribution. Limited samplings (cores) are used in laboratory experiments to determine all these properties.

Building a reservoir model, namely representing structure and rock and fluid properties, requires a complex set of software tools and data. Because of the limited resolution of such models, the limited understanding of reservoir processes, and the limited amount of data, such models are subject to considerable uncertainty. The modern approach is to build several (hundreds) of alternative reservoir models, which comes with its own set of challenges, in terms of both computation and storage. In addition, any prediction of flow and saturation changes (including the data that inform such changes such as 4D seismic and production data) requires running numerical implementation of multiphase flow, which depending on the kind of physics/chemistry represented (compressibility, gravity, compositional, reactive) may take hours to sometimes days.

1.2.3. The Challenge of Addressing Uncertainty

As production of oil/gas takes place in increasingly complex and financially risky situations, the traditional simple models of reservoir decline are gradually replaced by more comprehensive modeling of reservoir systems to understand better uncertainty in predictions made from such models. Based on the above description, Table 1.1 lists the various modeling components, subject to uncertainty, and the data involved in determining their uncertainty.

Despite the complexity in modeling, the target variables of such exercise are quite straightforward. In all, one can distinguish four categories of such prediction variables.

1. Volumes. How much target fluid is present? (a scalar)

2. *Recovery*. How much can be recovered over time under ideal conditions? (a time series)

3. *Wells*. Where should wells be placed and in what sequence? What strategy of drilling should be followed? Injectors/producer? Method of enhanced recovery? These are simply locations of wells and the time they will be drilled (a vector), and whether they are injecting or producing.

4. *Well controls*. How should wells produce? More complex wells are drilled, such as horizontal wells, that can be choked at certain points and their rates controlled in that fashion.

The primordial question is not necessarily the quantification of uncertainty of all the reservoir variables in Table 1.1 but of a decision-making process involving any of the target variables in question, which are

6 QUANTIFYING UNCERTAINTY IN SUBSURFACE SYSTEMS

Table 1.1	Overview	of the various	modeling	components,	fields of study,	, and data	sources for	UQ and	decision	making in
conventio	nal oil/gas	reservoirs.								

Туре	Class	Uncertain variable	Field of study	Main data	
Charge	Basin	Deposition, erosion	Basin and petroleum	Wells seismic core/	
	Source rock	Organic content; heat flow	system modeling,	log oil samples	
	Migration	Timing of kerogen transformation	- geochemistry		
		Amount			
	Faults	Location	Structural geology	Wells	
		Slip/throw			
		Transmissibility	Geomechanics	3D seismic	
Structural		Fractures			
Structural		Fault network hierarchy	Rock mechanics	Well tests	
	Horizons	Depth variation		Wells	
		Layer thickness variation	Stratigraphy	3D seismic	
	Contosto	WOC		Pressure data	
	Contacts	GOC	Hydrostatics		
	Posonuoir	Porosity		Core/log Seismic Production data	
		Permeability	– Carbonate geology		
	Reservoir	Lithology	_		
		Depositional system			
Petrophysical	Seismic	Velocity (P/S)	- Coismia processing	Seismic Core/logs	
		Density	Rock physics		
		Impedance (P/S)			
	Coor more housing	Poisson modulus	- Coomochanics	Coros	
	Geo-mechanics	Young's modulus	Geomechanics	Cores	
et - 1		PVT	Thermodynamics	Lab samples	
Fluid	Fluid	Relative permeability	Multiphase flow	Core experiments	
		Capillary pressure			

uncertain due to various reservoir uncertainties. Is the 2D seismic data warranting drilling exploration wells? Is there enough volume and sufficient recovery to go ahead with reservoir development? Which wells and where do we drill to optimize reservoir performance? To further constrain reservoir development, is there value in acquiring 4D seismic data and how? As such, there is a need to quantify uncertainty with these particular questions in mind.

1.2.4. The Libya Case

1.2.4.1. Geological Setting. To illustrate the various challenges in decision making under uncertainty for a realistic reservoir system, we consider a reservoir in the Sirte Basin in north central Libya. This system contains 1.7% of the world's proven oil reserves according to *Thomas* [1995]. Its geological setting as described by *Ahlbrandt et al.* [2005] considers the area to have been structurally

weakened due to alternating periods of uplift and subsidence originating in the Late Precambrian period, commencing with the Pan-African orogeny that consolidated several proto-continental fragments into an early Gondwanaland. Rifting is considered to have commenced in the Early Cretaceous period, peaked in the Late Cretaceous period, and ended in the early Cenozoic. The Late Cretaceous rifting event is characterized by formation of a sequence of northwest-trending horsts (raised fault blocks bounded by normal faults) and grabens (depressed fault blocks bounded by normal faults) that step progressively downward to the east. These horsts and grabens extend from onshore areas northward into a complex offshore terrene that includes the Ionian Sea abyssal plain to the northeast [Fiduk, 2009]. This structural complexity has important ramifications to reservoir development.

The N-97 field under consideration is located in the Western Hameimat Trough of the Sirte Basin (see Figure 1.2).



Figure 1.2 Structural elements of Sirte Basin. Schematic, structural cross-section from the Sarir Trough showing hydrocarbons in the Sarir Sandstone [*Ambrose*, 2000; *Ahlbrandt et al.*, 2005].

The reservoir under consideration, the WintersHall Concession C97-I, is a fault-bounded horst block with the Upper Sarir Formation sandstone reservoir. Complex interactions of dextral slip movements within the Cretaceous–Paleocene rift system have led to the compartmentalization of the reservoir [*Ahlbrandt et al.*, 2005].

Fluid flow across faults in such heterolithic reservoirs is particularly sensitive to the fault juxtaposition of sand layers. But the variable and uncertain shale content and diagenetic processes make estimation of the sealing capacity of faults difficult [*Bellmann et al.*, 2009]. Thus, faulting impacts fluid flow as well as fault sealing through fault juxtaposition of sand layers (see Figure 1.3).

1.2.4.2. Sources of Uncertainty. The reservoir is characterized by differential fluid contacts across the compartments. Higher aquifer pressure in the eastern compartment than the western compartment suggests the presence of either fully sealing faults or low transmissibility faults compartmentalization. However, the initial oil pressure is in equilibrium. Such behavior can be modeled using one of the two mechanisms:

1. a differential hydrodynamic aquifer drive from the east to the west, or

2. a perched aquifer in the eastern part of the field (see Figure 1.2).

By studying the physical properties of the fault-rock system such as pore-size distribution, permeability and capillary curves, the presence of only a single fault was falsified since that would not be able to explain the difference in the fluid contacts [*Bellmann et al.*, 2009]. When fault seal properties are modeled in conjunction with fault displacement, the cata-clastic fault seal is able to hold oil column heights across a single fault up to 350 ft. This indicates the presence of as many as four faults in the system. The displacement of all the faults is uncertain. This structural uncertainty in the reservoir in terms of the presence of faults and fluid flow across them needs to be addressed.

1.2.4.3. Three Decision Scenarios. Figure 1.4 shows three decision scenarios that are modeled to occur during the lifetime of this field.

Decision scenario 1. We consider the field has been in production for 5 years, currently with five producers. The field is operated under waterflooding. Waterflooding is an enhanced oil recovery method that consists of injecting water (brine) into the subsurface via injectors to push oil toward producers. At 800 days, one needs to address the question of increasing the efficiency of these injectors, by re-allocating rate between injectors. Evidently, the optimal re-allocation depends on the (uncertain) reservoir system. To determine this reallocation, the concept of injector efficiency is used. Injection efficiency models how well each injector aids production at the producing wells. This measure is calculated from a reservoir model (which is uncertain). The question is simple: How much needs to be re-allocated and where?



Figure 1.3 (a) Differential hydrodynamic trapping mechanism leading to different levels in fluid contact. (b) The perched aquifer explained as the reason. Contact levels depend on the number of faults in the system.



Figure 1.4 Three decision scenarios with three decision variables: injector efficiency, quality map, and production decline.

Decision scenario 2. At some point, optimizing just injectors will not cut it and new producing wells will need to be drilled, which comes at considerable cost. These wells should tap into un-swept areas of the reservoir system, for example, where the oil saturation is high. To do so, one often constructs "quality maps" [da Cruz et al., 2004], for example, maps of high oil saturations. These maps can then be used to suggest locations where this new well can be drilled. The question here is again straightforward: Where to drill a new producer?

Decision scenario 3. At the final stages of a reservoir life, production will need to be stopped when the field production falls below economic levels of current operating situations. This will depend on how fast production declines, which itself depends on the (uncertain) reservoir system. Companies need to plan for such phase, that is, determine when this will happen, to allocate the proper resources required for decommissioning. The question is again simple: What date to stop production?

The point made here is that the engineering of subsurface systems such as oil reservoir involves a larger number of fields expertise, expensive data, and possibly complex modeling, yet the question stated in these scenarios involve a simple answer: how much, where, when?

1.3. DECISION MAKING UNDER UNCERTAINTY FOR GROUNDWATER MANAGEMENT IN DENMARK

1.3.1. Groundwater Management Challenges under Global Change

Global change, in terms of climate, energy needs, population, and agriculture, will put considerable stress on freshwater supplies (IPCC reports, [Green et al., 2011; Oelkers et al., 2011; Srinivasan et al., 2012; Kløve et al., 2014]). Increasingly, the shift from freshwater resources toward groundwater resources put more emphasis on the proper management of such resources [Famiglietti, 2014]. Currently, groundwater represents the largest resources of freshwater accounting for one third of freshwater use globally [Siebert et al., 2010; Gleeson et al., 2015]. Lack of proper management where users maximize their own benefit at the detriment of the common good has led to problems of depletion and contamination, affecting ecosystems and human health, due to decreased water quality [Balakrishnan et al., 2003; Wada et al., 2010].

Solutions are sought to this tremendous challenge both in academia and in wider society. This requires a multidisciplinary approach involving often fragments of fields of science and expertise as diverse as climate science, land-use change, economic development, policy, decision science, optimization, eco-hydrology, hydrology, hydrogeology, geology, geophysics, geostatistics, multiphase flow, integrated modeling, and many more. Any assessment of the impact of policy and planning, change in groundwater use or allocation, will increasingly rely on integrated quantitative modeling and simulation based on understanding of the various processes involved, whether through economic, environmental, or subsurface modeling. Regardless of the complexity and sophistication of modeling, there is increased need for acquiring higher quality data for groundwater management. Computer models are only useful in simulating reality if such models are constrained by data informing that reality. Unfortunately, the acquisition of rigorous, systematic, high quality, and diverse data sources, as done in the petroleum industry, has not reached the same status in groundwater management, partly because such resources were often considered cheap or freely available. Data are needed both to map aquifers spatially (e.g., using geophysics) and to assess land use/land-use change (remote sensing), precipitation (remote sensing), hydraulic heads (wells), aquifer properties (pump tests), and heterogeneity (geological studies). It is likely that with an increased focus on the freshwater supply such lack of data and lack of constraints in computer modeling and prediction will gradually dwindle.

Quantitative groundwater management will play an increasing role on policy and decision making at various scales. Understanding the nature of the scale and the magnitude of the decision involved is important in deciding what quantitative tools should be used. For example, in modeling transboundary conflict [Blomquist and Ingram, 2003; Chermak et al., 2005; Alker, 2008; Tujchneider et al., 2013], it is unlikely that modeling of any local heterogeneity will have the largest impact because such problems are dominated by large-scale (read averaged) groundwater movement or changes and would rather benefit from an integrated hydro-economic, legal, and institutional approach [Harou and Lund, 2008; Harou et al., 2009; Maneta et al., 2009; Khan, 2010]. A smaller-scale modeling effort would be at the river or watershed scale where groundwater and surface water are managed as a single resource, by a single entity or decision maker, possibly accounting for impact on ecosystem, or land use [Feyen and Gorelick, 2004, 2005]. The impact of data acquisition and integrated modeling can be highly effective for resource management in particular in areas that are highly dependent on groundwater (such as the Danish case). In this context, there will be an increased need for making informed predictions, as well as optimization under uncertainty. Various sources of uncertainty present themselves in all modeling parameters, whether economical or geoscientific due to a lack of data and lack of full understanding of all processes, and their interactions.

In this book, we focus on the subsurface components of this problem with an eye on decision making under the various sources of subsurface uncertainty. Such uncertainty cannot be divorced from the larger framework of other uncertainties, decision variables or constraints, such as climate, environmental, logistical, and economic constraints, policy instruments, or water right structures. Subsurface groundwater management over the longer term, and possibly at larger scales, will be impacted by all these variables. Here we consider smaller-scale modeling (e.g., watershed) possibly over a shorter-term time span (e.g., years instead of decades).

Within this context, often, a simulation-optimization approach is advocated [Gorelick, 1983; Reed et al., 2013; Singh, 2014a, 2014b] where two types of problems are integrated: (i) engineering design, focusing on minimizing cost and maximizing extraction under certain constraints and (ii) hydro-economics to model the interface between hydrology and human behavior to evaluate the impact of policy. Such models require integrating the optimization method with integrated surface-subsurface models. The use of optimization methods under uncertainty (similar to reservoir engineering) is not within the scope of this book, although the methods developed can be readily plugged into such framework. Instead, we focus on smaller-scale engineering type, groundwater management decision analysis for a specific case, namely groundwater management in the country of Denmark.

1.3.2. The Danish Case

1.3.2.1. Overview. Groundwater management in Denmark is used as a backdrop to illustrate and present methods for decision analysis, uncertainty quantification, and their inherent challenges, as applied to aquifers. The Danish case is quite unique but perhaps also foretelling of the future of managing such resources through careful and dedicated top-down policy making, rigorous use of scientific tools, and most importantly investment in a rich and heterogeneous source of subsurface data to make management less of a guessing game.

Freshwater supply in Denmark is based on high-quality groundwater, thereby mitigating the need for expensive purification [Thomsen et al., 2004; Jørgensen and Stockmarr, 2009]. However, increasing pollution and sea-level changes (and hence seawater intrusion) have increased stresses on this important resource of Danish society. As a result, the Danish government approved a ten-point plan (see Table 1.2) to improve groundwater protection, of which one subarea consisted in drawing up a waterresources protection plan. The government delegated that 14 county councils be responsible for water-resources planning based on dense spatial mapping (using geophysics) and hydrogeological modeling as the basis for such protection. This high-level government policy therefore trickled down into mandates for local, site-specific, groundwater protection, a strategy and ensuing action
 Table 1.2
 Danish government's 10-point program from 1994.

Danish government's 10-point program (1994)
Pesticides dangerous to health and environment shall be removed from the market
Pesticide tax - the consumption of pesticides shall be halved
Nitrate pollution shall be halved before 2000
Organic farming shall be encouraged
Protection of areas of special interest for drinking water
New Soil Contamination Act – waste deposits shall be cleaned up
New Soil Contamination Act – waste deposits shall be cleaned up Increased afforestation and restoration of nature to protect groundwater
New Soil Contamination Act – waste deposits shall be cleaned up Increased afforestation and restoration of nature to protect groundwater Strengthening of the EU achievements
New Soil Contamination Act – waste deposits shall be cleaned up Increased afforestation and restoration of nature to protect groundwater Strengthening of the EU achievements Increased control of groundwater and drinking water quality
New Soil Contamination Act – waste deposits shall be cleaned up Increased afforestation and restoration of nature to protect groundwater Strengthening of the EU achievements Increased control of groundwater and drinking water quality Dialogue with the farmers and their organisations

Source: http://www.geus.dk/program-areas/water/denmark/ case_groundwaterprotection_print.pdf.

This structure has been changed since 1994. Denmark no longer has 14 counties but 5 regions. The regions are not directly involved in the groundwater protection, which now has been moved to state level, and the local management is controlled by municipalities.

plan (decision making) by local councils at the river/ watershed level.

The widespread availability of high-quality groundwater limits extensive pipeline construction. It was also recognized that some areas are more vulnerable to contamination from industry and agriculture than others; that despite extensive drilling, the aquifer heterogeneity and its impact on pumping could not be simply deduced or modeled from wells only. Hence, a more data-rich, modeling-intensive approach is required for proper management and to meet the goals in the government action plan. In that context, it was also established that simple drinking-well protection models based on multilevel radial protection zones ignored the impact of geological heterogeneity on how contaminants reach wells [Sonnenborg et al., 2015]. This is particularly relevant in Denmark where the shallow subsurface is largely dominated by the presence of "buried valleys." Buried valleys are mainly thought to be formed below the ice by erosion into the substratum caused by pressurized meltwater flow [Jørgensen and Sandersen, 2006]. Typically formed close to and perpendicular to the ice margin, these valleys often end abruptly, their cross-sections are typically U-shaped and can occur at a depth of up to 350 m. While the valleys are formed as isolated structures, they often show crosscutting relationships. Often younger valleys are eroded into the fill of older valleys, where these deposits are easily erodible than the surroundings. A complex network of



Figure 1.5 Location of the decision problem near the city of Kasted. The blue diamonds are the four alternative well locations (A, B, C, and D) in the decision problem. The grey lines are locations with SkyTEM data. Bottom: vertical profile of inverted SkyTEM data showing buried valleys.

cross-cutting valleys creates significant heterogeneity in the subsurface that influence groundwater recharge and flow. About half of the valleys are filled with hydraulic conductive sand, the rest filled with clayey deposits, but valleys with combined sand/clay infill are also quite common [*Sandersen and Jørgensen*, 2003]. Some of the valleys act as groundwater reservoirs, while others constitute barriers for groundwater flow/protection, making groundwater management unlikely to be reliable without any modeling or based on simple basic assumptions.

This geological phenomenon cannot be comprehensively modeled from boreholes only as such "point" information does not allow for an accurate mapping of the subsurface, leading to considerable uncertainty and risk in establishing protection zones.

Understanding the heterogeneity caused by the buried valleys depositional system is therefore critical to assessing aquifer vulnerability. Such valleys act as

underground "rivers," but such structure may themselves contain or act as flow-barriers created by the presence of clay [Refsgaard et al., 2010; Hoyer et al., 2015]. The complex intertwining of sand and clay makes such assessment difficult, and also because the majority of buried valleys are not recognizable from the terrain. In such depositional system, clay serves not only as a purifier, sand as a conduit, of water but also as a contaminant. This requires a comprehensive modeling of the various physical, chemical, and biological processes that take place in the heterogeneous subsurface. For that reason, a large geophysical data acquisition campaign was initiated, in particular through the use of various transient electro-magnetic (TEM) surveys [Møller et al., 2009] (see Figure 1.5). Such geophysical surveys provide a more detailed insight into the geological heterogeneity but their use does not necessarily result in a perfectly accurate map of the subsurface, due to limited resolution of the data source (similar to the limited resolution of seismic

data in reservoir modeling), limitations in data coverage, and the subjectivity of interpretations made from such data [*Jørgensen et al.*, 2013].

1.3.2.2. A Specific Decision Problem. Aquifer management requires dealing with conflicting objectives, uncertain predictions, limited data, and decision making within such context. At the local level, the decision to drill wells for drinking water extraction requires balancing the need for using resources versus the impact of extraction on the environment. In Denmark, the benefit of using aquifers for drinking water supply has to be weighed against the risk of (i) affecting streamflow, (ii) affecting wetland restoration, and (iii) risk of contamination from agriculture. These factors are related to EU regulations in which the Water Framework Directive is based.

We consider an area in Denmark, near the small town of Kasted, that requires considering such careful balancing act (see Figure 1.5). It has been observed that an extraction area is affecting wetlands; hence, in order to restore wetlands closer to their original state, a portion of the current groundwater abstraction will need to be re-allocated to a different area. Based on consideration of existing wells, current water distribution system, accessibility, and geological knowledge, four locations are proposed, A, B, C, and D, as shown in Figure 1.5. Jointly, the local municipality council and the water supply company must now decide on one of these locations. Evidently, we need to justify that the new location can indeed make up for the reduction in abstraction from the current well field, but also that this would not have any adverse effect on the environment, which would defeat the purpose of this re-allocation. We will treat this problem within a formal decision analytic framework using state-of-the-art groundwater modeling, sensitivity analysis, and uncertainty quantification.

Chapter 2 will introduce a formal decision analysis framework requiring stating objectives and using such objectives to compare stated alternatives on which decisions are based. This requires a formal statement of (i) what the alternatives are; no decision is better than the choice made from the stated alternatives, (ii) the objectives under which alternatives will be evaluated, typically in the form of "maximize this," "minimize that," and (iii) a quantitative measure of how well each alternative achieves the stated objectives (termed the "attribute"). Because of the existence of multiple competing objectives in this case, some statements of preferences are needed. In a decision analysis framework, these preferences are stated as value function, which transform preference to a common scale (e.g., 0-100). More details will be discussed in Chapter 2, more specifically,

the means of weighting the various conflicting objectives. Formally, we have constructed the following definitions:

1. *Alternatives*: the four locations/zones of pumping wells we are considering, assuming the well rates are fixed and known (corresponding to 20% of the abstraction at the existing well field). We could also consider several well rates.

2. Objectives: four objectives are stated:

• *minimize drawdown extraction*: preferably, the new location should bear the burden of the 20% extraction due to re-allocation and anything more is an additional plus. A large drawdown indicates poor aquifer conditions, and hence needs to be minimized.

• *maximize streamflow reduction potential*: depends on the flow in the stream given the existing abstraction, and the flow on the stream if we move 20% of the groundwater abstraction from the existing wells to the new well at any of the four locations.

• *maximize increased groundwater outflow to wetlands*: due to re-allocation, the aim is to restore the water table, thereby increasing the outflow of groundwater to the wetlands proximate to the existing well field.

• *minimize risk of contamination of drinking water*: the abstracted groundwater from the new well originates from within the so-called well catchment zone. This catchment zone intersects land use, such as "nature," "city," "farmland," and "industry." We aim to maximize the part of the well catchment that is located in nature and minimize that part of the catchment located within the category "industry" and "farmland." The city is considered as neutral.

The four target variables are calculated from a groundwater model, but because this model is uncertain, so are the payoffs associated with each target. This groundwater model has the following uncertain parameters (model components):

1. Uncertainty in the lithology distribution

2. Uncertainty in the hydraulic conductivity

3. Uncertainty on the boundary conditions

4. Uncertainty on the aquifer recharge

5. Uncertainty related to streams: connection with the aquifer (conductance) and digital elevation model (DEM) model used to define their elevation

To constrain this uncertainty, several data sources are available.

Conceptual geological understanding of buried valleys. The availability of dense borehole data in conjunction with high-quality geophysical data allows for a better understanding of the nature of the depositional system. Based on the large amount of studies in Denmark and neighboring areas [Sandersen and Jorgensen, 2003; Sandersen et al., 2009; Høyer et al., 2015], a conceptual model has been drawn (Figure 1.6), conveying the



Figure 1.6 Conceptual geological model (a sketch) of the buried valet deposits. Valleys are with different lithologies. Hence, hydraulic properties cross-cut each other [*Hoyer et al.*, 2015].

interpretation of the lithological architecture created by subsequent glaciation periods.

Hydraulic head observations. A Danish national well database, JUPITER [Møller et al., 2009], can be queried for measurements in the area of study. These measurements vary in quality, either because of how they are measured, type, and age of the borehole or because of the difference in coordinate and datum recording. A total of 364 head data were used in the study.

Stream discharge measurements were available from three gauging stations. Two stations had time series spanning approximately 20 years, while the third station had a span of 3 years.

Borehole data. The study area holds approximately 3000 boreholes with lithological logs of which the majority of boreholes are relatively shallow in depth (<50 m). Borehole information consists of lithology variation with depth. This data is also of different quality and based on metadata (drill-type, age) it is grouped into four quality groups.

Geophysical data. One of the defining features of the Danish groundwater management case is the availability of a rich and high-quality set of direct current (DC) and TEM geophysical data (see Figure 1.5). DC methods typically resolve the very shallow subsurface, while TEM methods resolve resistivity contrasts at greater depths. The TEM data were collected either through a port of numerous ground-based campaigns or through two campaigns (in 2003 and 2014) using the SkyTEM system [*Sørensen and Auken*, 2004] with the main purpose to delineate important buried valley structures, serving as

aquifers. Altogether, geophysical data collected in the area span 30 years, and 50 individual surveys, and they have all been stored in the national Danish geophysical database GERDA [*Møller et al.*, 2009].

The question now is simple: What is the best location to re-allocate drinking water, A, B, C, or D?

1.4. MONITORING SHALLOW GEOTHERMAL SYSTEMS IN BELGIUM

1.4.1. The Use of Low-Enthalpy Geothermal Systems

Low-enthalpy geothermal systems are increasingly used for climatization (heating/cooling) of buildings, in an effort to reduce the carbon footprint of this type of energy use. It is estimated [*Bayer et al.*, 2012] that the potential reduction of CO₂ emission reduction is around 30% compared to conventional systems. The main idea is the utilization of the subsurface, whether rocks, soils, saturated, or unsaturated, as a heat source or heat sink (cooling). To make this work in practice, two types of systems are used [*Stauffer et al.*, 2013] (see Figure 1.7).

1. *Closed systems* (BTES or borehole thermal energy storage): a series of vertical or horizontal pipes, often plastics, are installed in the subsurface. Fluids such as antifreeze solutions are circulated in the pipes to exchange heat with the subsurface. The system can be used for warming in winter and cooling in summer. Such systems are often installed in low-permeability soils, mitigating the risk of leakage of pipes.

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Figure 1.7 (a) An open (ATES) and (b) closed (BTES) shallow geothermal systems [Bonte, 2013].

2. Open systems (ATES or aquifer thermal energy storage): using drilling and boreholes, water is directly circulated between a production and an injection well through a heat exchanger (also called groundwater heat pump). Evidently, this requires a high-permeability subsurface. Heat stored in summer can theoretically be used in winter. However, because the open system is more sensitive to the ambient subsurface, its design needs to be done more carefully than a closed system. There is a risk that, if the system operates suboptimal, the energy stored cannot be fully recovered (e.g., in case of hydraulic gradient).

While the idea is straightforward, the practical implementation raises a number of important questions. Next to the evident question on how to design the system, questions related to the impact of such thermal perturbation on the subsurface system need to be addressed. These impacts are multifold:

1. *Hydrological*. Changes in temperature induces a heat flux, which may affect areas further away from wells (the thermally affected zone). Catchment areas of existing drinking water wells may be affected, which in turn may impact flow and hence such change increases the risk for unwanted (and unforeseen) contamination or cross-aquifer flow.

2. *Thermal.* A long-term warming or cooling may occur. This may cause interference with other uses of groundwater. In addition, it may affect the performance of the system because of possible freezing or short-circuiting the heat exchange. This thermal impact needs to be considered jointly with other long-term sources of thermal changes such as climate change and urbanization.

3. *Chemical*. Rainwater is filtrated in the subsurface and such a process produces fresh drinking water, leading to a specific vertical groundwater stratification with shallow oxidized, nitrate-rich groundwater and reduced iron-rich deeper water. ATES can introduce a mixing that affects

the quality of the groundwater. In addition, one needs to be concerned of other effects such as change in reaction kinetics, organic matter oxidation, and mineral solubility. Urban areas are already vulnerable to contamination from various pollution sources and chemical changes may further enhance that effect.

4. *Microbial.* The groundwater system is an ecosystem (consisting of bacteria, fungi, pathogens, and nutrients). Any temperature changes may affect this system, and hence affect the balance of this ecosystem, possibly leading to changes in water quality. In addition, microbial changes may lead to clogging of this system, which is particularly relevant near boreholes.

Since exploitation of the subsurface for heat will add an additional stress to a system already subject to stresses from other sources, such as drinking water extraction, contaminants, and geotechnical construction, it is likely that new policies and regulations will need to address the shared use of this resource. Such regulations are likely to include monitoring (perhaps in the same sense as required for CO_2 sequestration) to mitigate risk or reduce the impact of the thermal footprint. Next we discuss the design of such monitoring system and what affect the unknown subsurface properties have on that design. Then, we introduce a specific case of data acquired in an aquifer in Belgium.

1.4.2. Monitoring by Means of Geophysical Surveys

1.4.2.1. Why Geophysics?. The design as well as monitoring of the shallow geothermal system, like many other subsurface applications, require a multidisciplinary approach, involving several fields such as geology, hydrogeology, physics, chemistry, hydraulics engineering design, and economics. For example, *Blum et al.* [2011] showed (based on systems in Germany) that subsurface characteristics are insufficiently considered for a proper

design. Characterization of heat flow, temperature changes, and its effect on the ambient environment requires characterizing geological heterogeneity, combined fluid and thermal properties, as well as geochemical characteristics (to study impact on subsurface chemistry). Early models relied mostly on analytical equations. However, such approaches ignore the complexity of the subsurface and the observed (see later) heterogeneity of temperature and temperature changes in the subsurface, leading to inadequate design. The more modern approach relies on creating groundwater models and modeling combined fluid flow and heat transport using numerical simulators. Next to traditional tests such as borehole flowmeter tests, slug tests, hydraulic pumping tests, and tracers, two field experiments are used to constrain the thermal parameters required for such simulators: the thermal response test (TRT) and the thermal tracer test (TTT). These are used to characterize thermal diffusivities and hydraulic and thermal conductivities required for simulations. These values can be obtained both from field and from laboratory data. However, both TRT and TTT are borehole centric tests. For example, with a TRT one circulates a hot fluid and continuously measures temperature changes of the fluid. TTT involved two wells and works like a tracer but now for heat. Such experiments can be short or long term (short = hours, long = months). In the short-term experiments, heated or cooled water is injected as a tracer, and temperature changes are measured in a nearby observation well. To derive the required properties, one can either use analytical equations (relying on simplifying assumptions) or build numerical models and solve inverse problems. There are several problems that arise when limiting oneself to only these types of test. First, they provide only information near the well (TRT) or between well locations. Second, geological heterogeneity makes

direct interpretation difficult for such tests and hence inverse modeling becomes tedious.

New techniques are therefore needed to more directly and more effectively monitor the spatial and temporal distributions of temperature in the system which could lead to (i) better design the geothermal system and the monitoring network, (ii) prevent any thermal feedback/ recycling, and (iii) image and control the thermal affected zone [*Hermans et al.*, 2014]. Here we focus on the use of a specific method, namely electrical resistivity tomography (ERT) and its time-lapse variety to characterize temperature and its changes under shallow geothermal exploitation and monitoring.

1.4.2.2. ERT and Time-Lapse ERT. ERT is a method that images the bulk electrical resistivity distribution of the subsurface (Figure 1.8). Electrical resistivity depends on several properties of relevance for shallow geothermal systems: (i) clay mineral content, (ii) water saturation and salinity, (iii) porosity, and (iv) temperature. As with any geophysical technique, the target physical property (temperature here) needs to be untangled from other influences. Consequently, because of geological heterogeneity, this becomes more difficult to achieve and requires knowledge of such heterogeneity as well as the various rock physics relations between the properties involved.

Practically, electrical currents are injected between two current electrodes, either on the surface or in the borehole. Then, the resulting potential difference is measured simultaneously between two different (potential) electrodes. Because the current is known (a control), the ratio between the measured difference of electrical potentials equals the electrical resistance, as follows directly from Ohm's law. This process is repeated along one or several profiles using many quadrupoles to acquire 2D or 3D datasets. The acquired values of electrical resistance



Figure 1.8 The use of electrical resistivity tomography in the design of shallow geothermal systems. From Hermans et al. [2014].



Figure 1.9 Example of temperature monitoring during a heat-tracing experiment from ERT. Modified after Hermans et al. [2015].

measured at each (quadrupole) location needs to be inverted into an electrical resistivity distribution that can then be linked to a target physical property (e.g., temperature).

Monitoring is a time-varying study; hence, instead of taking one snapshot (in time), ERT imaging can be repeated to detect changes. Inversion into electrical resistivity is repeated and compared with the base survey. Similar to the static inversion, changes in electrical resistivity can be related to changes in target physical properties such as temperature changes. One of the advantage of time-lapse ERT as applied to geothermal monitoring is that temperature is the dominant change; hence, time-lapse ERT becomes easier to interpret in terms of temperature, as other effects are mostly constant. As an example, Hermans et al. [2015] monitored a heat-tracing experiment with cross-borehole ERT. Assuming no changes in chemistry and the absence of clayey minerals, Hermans et al. were able to image from ERT changes in temperature as low as 1.2°C with a resolution of a few tenths of degree Celcius (Figure 1.9).

1.4.2.3. *Issues.* Despite the straightforward advantage of ERT and its time-lapse variety, several challenges occur because of non-ideal conditions in the subsurface and in performing such surveys.

Smoothing. As with any geophysical technique, ERT data provides only a smooth view of the physical properties of the subsurface. As a result, any inversion of such data is non-unique (see Chapter 6 on inverse modeling). However, most current approaches rely on some smooth inversion (using regularization terms, see Chapter 6). The lack of proper representation of actual subsurface variability has led to poor recovery of mass-balance in tracing experiments [Singha and Gorelick, 2005; Muller et al., 2010] and over- or underestimation of the physical properties due to over-smoothing of the geophysical image [Vanderborght et al., 2005; Hermans et al., 2015]. Additionally, to convert electrical resistivity changes to temperature changes, one needs to rely on petrophysical relationships established in small-scale laboratory experiments that become difficult to apply (without error) to the larger-scale inversions. Such approaches will work in relatively homogeneous deposits but lose their applicability in more heterogeneous systems. In Chapter 6, we show how standard regularization methods do not lead to an adequate quantification of the uncertainty in the obtained temperature changes. Such an uncertainty is needed for risk quantification in the design of the system.

Noise. Noise in ERT measurements is composed of a random and a systematic component. The latter may be correlated in time. Random error arises from variations in the contact between the electrodes and the ground [Slater et al., 2000]. Systematic errors are related to the data acquisition, hence any problems with electrode placement (e.g., misplaced, disconnected). Time-lapse geophysical measurements are subject to the repeatability issues, namely that exact same conditions and configurations need to occur over time, which is rarely the case. One way to address noise is to make use of the so-called reciprocal measurements, which involves reversing the current and potential electrodes. Under ideal, non-noise conditions, this should result in identical readings. It is often observed that the error obtained by means of reciprocal measurement increases with resistance.

1.4.2.4. Field Case. We consider a specific field case where geophysical data is used to assess the potential for a geothermal heat exchanger for building heating. The aim is to assess whether an alluvial aquifer allows storing thermal energy and restore it at a later stage. The aim is therefore to predict heat storage capacity of the system undergoing an injection and pumping cycle. Here we study one such cycle of injecting hot water for 30 days, then extracting for 30 days. In other words, the target is to predict the change in temperate during extraction. This quantifies the efficiency of the recovery and aids