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The Earth Resources Challenge

Co-Authored by: Troels Norvin Vilhelmsen¹, Kate Maher², Carla Da Silva³, Thomas Hermans⁴, Ognjen Grujic⁵, Jihoon Park⁵, and Guang Yang⁵

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 Shepherd. 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 CO₂), is often called the blue energy toward a green future. 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 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, CO₂, 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 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

\[ \text{Volume} = \text{area} \times \text{thickness} \times \text{porosity} \times \text{oil saturation} \times \text{formation volume factor} \]

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...
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/producers? 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
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 terrane 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 re-allocation, 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](image-url)  
**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](image-url)  
**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., 2012; Gleson 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; Gleson 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, multi-phase 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 water-resources 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 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 [Sørensen 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

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<th>Table 1.2 Danish government’s 10-point program from 1994.</th>
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<td><strong>Danish government’s 10-point program (1994)</strong></td>
</tr>
<tr>
<td>Pesticides dangerous to health and environment shall be</td>
</tr>
<tr>
<td>removed from the market</td>
</tr>
<tr>
<td>Pesticide tax – the consumption of pesticides shall be</td>
</tr>
<tr>
<td>halved</td>
</tr>
<tr>
<td>Nitrate pollution shall be halved before 2000</td>
</tr>
<tr>
<td>Organic farming shall be encouraged</td>
</tr>
<tr>
<td>Protection of areas of special interest for drinking water</td>
</tr>
<tr>
<td>New Soil Contamination Act – waste deposits shall be</td>
</tr>
<tr>
<td>cleaned up</td>
</tr>
<tr>
<td>Increased afforestation and restoration of nature to protect groundwater</td>
</tr>
<tr>
<td>Increased control of groundwater and drinking water quality</td>
</tr>
<tr>
<td>Dialogue with the farmers and their organisations</td>
</tr>
</tbody>
</table>

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 comprehen-
sively 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 accu-
rate map of the subsurface, due to limited resolution of the
data source (similar to the limited resolution of seismic

---

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.
data in reservoir modeling), limitations in data coverage, and the subjectivity of interpretations made from such data [Jorgensen 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 Jørgensen, 2003; Sandersen et al., 2009; Hoyer et al., 2015], a conceptual model has been drawn (Figure 1.6), conveying the
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.
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](image_url)
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 advantages 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 temperature during extraction. This quantifies the efficiency of the recovery and aids
in the design of the heat pump. The target for prediction is a simple function of time: $\Delta T(t)$.

The study site is located in the alluvial aquifer of the Meuse River in Hermalle-sous-Argenteau, Belgium, consisting of a 10 m thick zone. The water level is located at 3.2 m depth. Based on borehole logs, the saturated deposits can be divided into two distinct layers. The upper layer, between 3 and about 7 m depth, is composed of gravel in a sandy matrix. The bottom layer is composed of coarse clean gravel. The bedrock composed of low permeability carboniferous shale and sandstones lies at 10 m depth and constitutes the basement of the alluvial aquifer. The reader can refer to Klepikova et al. [2016] and Hermans et al. [2015] for more details on the site.

For 30 days, heated water is continuously injected into a well at a rate of 3 m$^3$/h. The temperature of the injected water is 10°C above the background temperature. At the end of the 30-day period, water is extracted from the well at the same rate of 3 m$^3$/h. The change in temperature of the pumped water compared to the initial value in the aquifer (i.e., before injection) is recorded for another 30-day period. The thermal energy recovery can be estimated using the temperature of the extracted water. The simulation is limited in time to avoid considering changing boundary conditions with time. Similarly, a rate of 3 m$^3$/h allows to reduce the size of the investigated zone.

In Chapter 8, we will address the following questions:
1. In the design of this specific system, which model parameter most impacts the prediction of $\Delta T(t)$. Many uncertainties exist as discussed earlier; hence, we need to focus on those that matter.
2. What data can be used to narrow those model uncertainties that most impact the decision variable, here $\Delta T(t)$. Will it be useful to use ERT data?
3. If we would decide to go ahead with acquiring ERT data, how would the uncertainty on $\Delta T(t)$ be reduced?
4. Given that we are working in such a complex system, is there a way to test our various modeling assumptions (meaning aiming to falsify them, see Chapter 5)?

1.5. DESIGNING STRATEGIES FOR URANIUM REMEDIATION IN THE UNITED STATES

1.5.1. Global Environmental Challenges

Similar to the need to protect and manage groundwater resources in the next century, stresses on the environment, due to anthropogenic activities, will continue to grow. For example, the United States government, under the Department of Energy (DOE), formulated the explicitly stated goals of developing sustainable solutions to such environmental challenges, based on a predictive understanding of environmental systems. Some of the stated goals are as follows: (i) synthesize new process knowledge and innovative computational methods that advance next generation, integrated models of the human–Earth system; (ii) develop, test, and simulate process-level understanding of atmospheric systems and terrestrial ecosystems, extending from bedrock to the top of the vegetative canopy; (iii) advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable systems-level prediction and control; and (iv) identify and address science gaps that limit translation of fundamental science into solutions for the most pressing environmental challenges (http://science.energy.gov/ber/research/cesd/).

As in the groundwater case, there is a need to understand and study watersheds as complex hydrobiogeochemical systems, in particular how such systems respond to contaminant loading. This systems approach is similar to the “reservoir system” or the “groundwater system.” However, now an additional set of processes may complicate matters. For example, an understanding of the complex processes and interactions that occur from bedrock to the top of the canopy is necessary [Brantley et al., 2007]. This requires modeling and understanding processes from the molecular to a planet-wide scale of perturbations or changes. The latter has led to the building of mechanistic (numerical models) reactive transport models. Such models incorporate knowledge of microbial processes, speciation, and interactions of inorganic elements with microbes, and how these processes act on different time and space scales [Li et al., 2017].

These broad scientific questions are often addressed within specific decision-making frameworks and policy outcomes in mind. Hence, there is a need to integrate these various processes within a single framework, to provide guidance on what data should be collected to adhere to regulations, to design any remediation strategy, and to ultimately monitor and verify the effects of such remediation.

1.5.2. Remediation: Decision Making Under Uncertainty

On a more local scale, there will be an increased need to remediate contaminated soils or groundwater that may pose a significant risk to human health. Decision making for contaminant remediation may well be more complex than for petroleum or (uncontaminated) groundwater systems. Such a decision making varies highly by country, regions, or even state (see Table 1.3). For example, at an EPA Superfund site near Davis, California, three lead agencies oversee the cleanup of chemical spills: the Central Valley Regional Water Quality Control Board (RWQB), the California Department of Toxic Substances
18 QUANTIFYING UNCERTAINTY IN SUBSURFACE SYSTEMS

Table 1.3 Example of stakeholders in the decision context of contamination remediation.

<table>
<thead>
<tr>
<th>Facility owner</th>
<th>Regulatory agencies</th>
<th>Local/county agencies</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Achieve regulatory compliance</td>
<td>• Protect human health and the environment, including groundwater resources</td>
<td>• Optimize zoning</td>
</tr>
<tr>
<td>• Utilize risk-based techniques</td>
<td>• Protect groundwater resources</td>
<td>• Maximize tax revenues</td>
</tr>
<tr>
<td>• Minimize/eliminate disruption of operations</td>
<td>• Achieve regulatory compliance</td>
<td>• Accelerate schedule</td>
</tr>
<tr>
<td>• Minimize costs</td>
<td>• Eliminate off-site impacts to receptors</td>
<td>• Protect human health and the environment</td>
</tr>
<tr>
<td>• Reduce long-term treatment and liabilities</td>
<td>• Involve stakeholders</td>
<td>• Maximize quality of life</td>
</tr>
<tr>
<td></td>
<td>• Maintain reasonable schedule</td>
<td>• Protect groundwater resources</td>
</tr>
<tr>
<td></td>
<td>• Obtain reimbursement for oversight costs</td>
<td></td>
</tr>
</tbody>
</table>

Source: Adapted from “A decision-making framework for cleanup of sites impacted with light non-aqueous phase liquids (LNAPL)” (2005)

Control, and the US EPA (United Stated Environmental Protection Agency). Often environmental consultants are hired by responsible parties (here UC Davis and the DOE), leaving the decisions on which remedial options to consider. Recommendations are made to the lead agencies for implementation and final decision making.

Within this context, the US EPA guidelines are outlined in a document entitled “A decision-making framework for cleanup of sites impacted with light non-aqueous phase liquids (LNAPL)” (2005). Although specific to LNAPL, the document is only a guide (not a policy or legal requirement), aiming to provide practicable and reasonable approaches for management of petroleum hydrocarbons in the subsurface (and hence is specific to contamination from petroleum product around refineries, pipelines, etc.). Although not based on any formal decision analysis (such as in Chapter 3), the document outlines the complex interaction of stake holders (oil industry, local communities, government agencies), formulation of high-level goals and objectives, the implementation of remediation strategies, modeling of potential exposure pathways, and data acquisition. This decision process involves different parties with different competing objectives. The treatment of these competing objectives within a formal decision-making process will be discussed in Chapter 2.

1.5.3. Remediation: Data and Modeling

Targeted data collection is critical to the evaluation of several remediation options and the selection of the most appropriate alternative for a given site, as many alternatives may present themselves such as “clean up the site to pristine conditions,” and “clean only the most impacted portions and contain the remainder of the contamination on site.” A decision will ultimately consist of choosing among these alternatives (and accompanied remediation methods) based on the stated objectives. Similar to the groundwater case, data and modeling will have value as long as they inform the “payoffs” for each alternative. If all aspects of the subsurface are clearly informed, the effect of remediation would be perfectly known, then a decision is simply made from the highest payoff (or lowest cost). However, because of the various uncertainties involved, decisions will need to be made under uncertainty.

The importance of prediction of contaminant distribution in space and time through numerical modeling has long been acknowledged [Wagner and Gorelick, 1987; Morgan et al., 1993; Andrićević and Cvetković, 1996; James and Oldenburg, 1997; Maxwell et al., 1999]. Such a prediction is especially important toward designing and evaluating remediation strategies. For example, in one mercury contamination remediation case study, various risk assessment/prediction tools are developed to evaluate options of active management such as capping and dredging, or passive natural attenuation [Wang et al., 2004]. As monitoring costs are very expensive and such monitoring data provide only a short-term inference on future events within a limited spatial area, numerical modeling is needed to provide meaningful long-term predictions. Behavior of contaminant plumes, both conservative and reactive, has been studied extensively both at the lab-scale and at the field-scale experiments, to assist developing better numerical modeling tools that provide these predictions [Lovley et al., 1991; Yabusaki et al., 2007; Li et al., 2011; Williams et al., 2011]. However, uncertainties are naturally associated with numerical modeling. Such uncertainties in models of contaminant transport come from spatially variable hydraulic properties, physical and chemical descriptions or the initial and boundary conditions, knowledge of the contaminant source, and importantly the rates and mechanisms associated with the physical and biochemical processes.

As decisions made in contaminant remediation depend on long-term predictions within a small tolerance range, efforts have been made across research areas, such as hydrogeology, geology, geostatistics, geophysics, biogeochemistry, and numerical modeling, to create better models that improve accuracy and reduce the uncertainties of predictions [Cirpka and Kitamidis, 2000; Sassen et al.,...
More recently, there have been rising concerns over remediation solutions to real-world, polluted groundwater systems. Such contaminations were caused by destructive human activities during the 20th century [Wang et al., 2004; Yabusaki et al., 2007; Chen et al., 2012].

1.5.4. Uranium Contamination in the United States

In this book, we will be concerned with groundwater contamination resulting from the extraction and processing of uranium ore during the Cold War era that poses environmental risk across hundreds of sites in the United States, particularly within the upper Colorado River Basin [Palmisano and Hazen, 2003]. A US DOE site near Rifle, Colorado, contains a contaminated floodplain that has been the focus of detailed investigation [as reviewed in Anderson et al., 2003; Williams et al., 2009, 2011; Orozco et al., 2011]. The site once contained a milling facility for ores rich in uranium and other redox sensitive metals (e.g., vanadium, selenium, and arsenic). After removal of the contaminated overburden, low but persistent levels of contamination within subsurface sediments still affect groundwater quality and flow directly to the Colorado River. Elevated concentrations of contaminants can be harmful to young-of-year fish that use the backwater channels as habitat during late summer. The Rifle site is also within the above described wider context of building models to quantify how land use and climate change affect subsurface carbon fluxes and transformations, flow paths, subsurface microbial communities, and ultimately the biogeochemical behavior of a watershed. The wealth of data collected at this site provides a testbed for developing such models, testing hypotheses, generating predictive uncertainty, and ultimately quantitative prediction of short- and long-term evolution of this biogeochemical system [Williams et al., 2011; Zachara et al., 2013; see also Williams et al., 2013].

Acetate injection has been evaluated at the Rifle pilot site to examine the effectiveness of in situ bio-remediation [Yabusaki et al., 2007; Li et al., 2011; Williams et al., 2011]. The acetate amendment stimulates the indigenous dissimilatory iron reducing microorganisms to catalyze the reduction of U(VI) in groundwater to insoluble U(IV) [Lovley et al., 1991] and offers a cost-effective, in situ remediation solution.

1.5.5. Assessing Remediation Efficacy

To study the efficacy of acetate injection as a remediation strategy, four field bio-stimulation experiments have been conducted at the US DOE’s Integrated Field Research Challenge site in Rifle, Colorado, as shown in Figure 1.10. Previous experiments have shown that acetate injection is capable of immobilizing uranium [Li et al., 2010; Williams et al., 2011]. Figure 1.11 shows...
the setup of the 2007 Winchester experiment, which is the data we will be using in this book. Acetate mixed with conservative tracer is injected into a set of injector wells. Concentrations of tracers as well as acetate, sulfate, and \( \text{UO}_2^{2+} \) are measured at observation wells. The goal of this study is to predict the volume of immobilized uranium, since this will indicate the efficacy of the injection experiment.

The uncertainties associated with predicting the extent of uranium immobilization are substantial. Similar to the case of shallow geothermal monitoring, the amount of data (even at these kinds of sites) remains limited (although geophysical surveys have also been conducted at these sites) [Williams et al., 2009; Orozco et al., 2011]. We distinguish three groups of uncertainties:

1. **Geological.** This pertains to the uncertain hydraulic conductivity and porosity, their statistical properties and spatial variability.

2. **Biogeochemical.** This pertains to the various geochemical reactions taking place upon acetate injection, in particular the kinetics of such reactions, as well as the initial concentrations and volumes and surface areas of iron-bearing minerals.

3. **Hydrological.** This pertains to the various boundary conditions such as hydraulic gradients, recharge, and so on.

Therefore, the questions are as follows:

1. Which of all these uncertainties impacts most the remediation efficacy?

2. Having this knowledge, how much can we predict long-term efficacy from short-term tracer monitoring?

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**1.6. DEVELOPING SHALE PLAYS IN NORTH AMERICA**

**1.6.1. Introduction**

A new and vast source of energy, organically rich shale rocks, has changed the global energy landscape in the last decade (see Figure 1.12). Development of such resources is very complex and relies on substantial amount of drilling (operators drill hundreds of wells per year). Decision questions regarding shale systems are not very different from those in conventional systems: Where to drill? How to fracture the rock? What production to expect? However, the well-established approaches developed for conventional reservoirs are not readily applicable to shales, mainly due to the rapid development of these plays. Unconventional wells are drilled at a rate of several wells per week, while one comprehensive prediction and uncertainty quantification could take anywhere from a few weeks to several months. This peculiar nature of unconventional reservoirs calls for the development of new, rapid and comprehensive data analysis and uncertainty quantification methods. In that sense, the problems described in this section are unique and the methods different from those introduced in the previous applications fields. Here statistical and machine learning methods appeared to be more attractive because of their rapid learning and prediction. However, this learning is challenging, involving spatial, temporal, and multivariate elements of high degrees of complexities.
1.6.2. What are Shales Reservoirs and How are They Produced?

In oceans, a large amount of organic matter from microorganisms and planktons falls to the seabed and mixes with silt, clay, and other materials already present, forming an organic source. Sediment inflow from rivers brings clastic material that is simply deposited on top of the organic source, further burying sediments into the subsurface. Over the course of millions of years, such organically rich and finely grained mixture turns into a specific type of rock, shale, and ends up buried at very large depths. Large depth means large overburden, which imposes high pressures on the organically rich shale, hence increasing its overall temperature. When the temperature of the shale exceeds 120°C the organic matter starts to “cook.” Hydrocarbon molecules start forming from the organic matter already contained within the rock. When the volume of hydrocarbons in the rock becomes critical, low density and buoyant forces push hydrocarbons toward the shallower zones of the subsurface (toward lower pressure) in a process called “migration.” Normally, hydrocarbons would migrate all the way to the surface (seeping holes); however, they often end up trapped in highly porous sandstones forming hydrocarbon reservoirs. These hydrocarbon reservoirs are also known as the conventional reservoirs, while the organically rich shale that generated the hydrocarbons is commonly referred to as the “source rock.”

The amount of hydrocarbons contained in conventional reservoirs is only a small portion of the oil that the source rocks originally generated. Source rocks still contain a large amount of immobile hydrocarbons and as such represent a potentially large energy resource. Every shale rock is different, and the way in which it bounds with the hydrocarbons is also different. This bounding is a result of complex interplay of the rock and fluid compositions and complex physical interactions. Some shales are capable of chemically absorbing gas (sorption), while others are not, sometimes the viscosity of oil is high, and sometimes it is low. Some shales are very brittle with dense networks of natural fractures, while some others are very ductile with almost no natural fractures. What all shales have in common is the fact that they are all almost impermeable and highly organically rich rocks.

Early efforts to produce shale reservoirs through vertical drilling and completion have mostly resulted in failure, due the low permeability of shales. However, with the advent of hydraulic fracturing (HF) and in some cases usage of explosives, production of commercial quantities of hydrocarbons at specific shale plays was possible. The most notable ones are the Big Sandy gas field in Eastern Kentucky, North part of the Marcellus shale in the state of New York where some wells were drilled in the early
1800s (indeed almost 200 years ago), and New Albany shale. These sporadic successes were later attributed to the very well developed networks of natural fractures (producing high permeability flow paths). Real, organized, large-scale effort to tap into shales did not occur until the first big oil crisis in the late 1970s when US DOE initiated the game-changing Eastern Shales Gas Project (ESGS). This project is the largest research project ever taken on shale reservoirs whose successful result is best reflected on US independence on foreign oil at present. ESGS identified that horizontal drilling technology with multistage fracturing is a technique capable of unlocking the potential of organically rich shales. The idea is simple, try to maximize the contact between the well and the rock by producing as many as possible artificial flow paths/fractures.

Today, operators drill long horizontal wells (several thousands of feet long) and conduct massive HF jobs with anywhere between 10 and 40 man-made hydraulic fractures (commonly referred to as “stages”) (see Figure 1.13). HF is a complicated and expensive procedure with many different parameters whose complex interplay with the geology determines the quality of the produced hydraulic fractures and ultimately affects the hydrocarbon production. Table 1.4 provides just a few of the many engineering and geological parameters involved. (The abbreviations given in the last column of the table will be used in Chapter 8.) Obviously, optimization of such parameters achieves significant cost reductions, hence maximizes profit. Given that every shale is different, best fracturing practices identified in one shale play do not necessarily translate directly as the most optimal to other shale plays. Therefore, every shale play data are analyzed independently with the aim to understand production, interplay between HF and geology, and ultimately use such understanding to produce some forecasting models. All this in an effort to answer the simple business questions: where to drill, how to complete, and what to expect?

Analysis of data from shale production is not a trivial endeavor. First, the input data (covariates) are very high dimensional (see Table 1.4), making standard statistical techniques difficult to apply. Second, production data from different wells comprise of time series, but of different time intervals, depending on how long the well has been in production. In Chapter 8, we will consider two real field cases, one from the Barnett shale with thousands of wells and one from newly developed system with only 172 hydraulically fractured horizontal wells.
1.6.3. Shale Development Using Data Science

Examples of data centric modeling for shales are in Mohaghegh et al. [2011] who utilized artificial intelligence to data mine and forecast production in unconventional reservoirs (see also Bhattacharya and Nikolaou [2013]). Most of these methods predict scalar values, such as a rate at a given time. However, decision variables in shale systems are rates or volumes of produced hydrocarbons as they vary over time. Therefore, understanding shales and identifying value-creating practices with data-driven techniques require proper handling of production time series. This is often challenging since production time series come as noisy, discrete observations of production rates over time. In addition, any data scientific method will need to account for the large number of variables involved as well as the spatial heterogeneity of the shale play itself, leading to spatial variation of production, even if they would be produced under the exact same engineering conditions.

Shale management from exploration and production comes with a large series of problems and questions. Here we will focus on those that pertain to the use of data science to predict and quantify uncertainty to what happens when the play is in production. As more wells are drilled and produced, more data become available about geological parameters, completion parameters, and production decline.

The following are the questions we will be most interested in:

1. Which geological and completion parameters most impact production? This a question of sensitivity and it is needed to make the high-dimensional problem manageable before developing any prediction or UQ methods.
2. How to predict and quantify uncertainty on production decline in a new well for given geological and completion parameters? This question requires building a statistical relationship between several covariates and an uncertain function.
3. How many wells need to be in production before a statistical model can confidently estimate production decline.

<table>
<thead>
<tr>
<th>Type of uncertainty</th>
<th>Parameter</th>
<th>Unit</th>
<th>Abbreviation</th>
</tr>
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<tbody>
<tr>
<td>TARGET</td>
<td>Production</td>
<td>Oil rates</td>
<td>stb/day</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Gas rates</td>
<td>stb/day</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water rates</td>
<td>stb/day</td>
</tr>
<tr>
<td>Completions</td>
<td>Number of completion stages</td>
<td>#</td>
<td>CMP STAGES STIMULATED</td>
</tr>
<tr>
<td></td>
<td>Total amount of injected fluid</td>
<td>gal</td>
<td>CMP TOTAL FLUID PUMPED GAL</td>
</tr>
<tr>
<td></td>
<td>Total amount of injected proppant</td>
<td>lbs</td>
<td>CMP TOTAL PROPPANT USED</td>
</tr>
<tr>
<td></td>
<td>Stimulated lateral length</td>
<td>ft</td>
<td>CMP STIMULATED LATERAL LENGTH</td>
</tr>
<tr>
<td></td>
<td>Total amount of slick water</td>
<td>bbl</td>
<td>CMP AMT SLICKWATER BBL</td>
</tr>
<tr>
<td></td>
<td>Total amount of injected x-link fluid</td>
<td>bbl</td>
<td>CMP AMT CROSSLINK BBL</td>
</tr>
<tr>
<td></td>
<td>Completion stage interval</td>
<td>ft</td>
<td>CompStageInterval</td>
</tr>
<tr>
<td></td>
<td>Total amount of linear fluid</td>
<td>bbl</td>
<td>CMP AMT LINEAR BBL</td>
</tr>
<tr>
<td>Geographical</td>
<td>X location</td>
<td>ft</td>
<td>GeolX Rel</td>
</tr>
<tr>
<td></td>
<td>Y location</td>
<td>ft</td>
<td>GeolY Rel</td>
</tr>
<tr>
<td></td>
<td>Z location (depth)</td>
<td>ft</td>
<td>GeolZ</td>
</tr>
<tr>
<td>PVT</td>
<td>Oil API gravity</td>
<td>api units</td>
<td>GeolAPIGrav</td>
</tr>
<tr>
<td>Petrophysical</td>
<td>Total organic content (TOC)</td>
<td>%</td>
<td>PetroTOC</td>
</tr>
<tr>
<td></td>
<td>Clay content</td>
<td>%</td>
<td>PetroVClay</td>
</tr>
<tr>
<td></td>
<td>Water saturation</td>
<td>%</td>
<td>PetroSwt</td>
</tr>
<tr>
<td></td>
<td>Porosity</td>
<td>%</td>
<td>PetroPor</td>
</tr>
<tr>
<td></td>
<td>Total amount of quartz</td>
<td>%</td>
<td>PetroVQtz</td>
</tr>
<tr>
<td></td>
<td>Amount of pyrite</td>
<td>%</td>
<td>PetroPyr</td>
</tr>
</tbody>
</table>

Table 1.4 Overview of some of the parameters involved in designing unconventional shale operations.
in a new location? With too few data, data scientific method will fail to produce meaningful prediction because uncertainty is too large.

1.7. SYNTHESIS: DATA–MODEL–PREDICTION–DECISION

While the various applications of prediction and UQ are quite diverse, there are various common elements that are useful in summarizing. To do this, let us consider the following statements, including some additional comments.

In engineering the subsurface, uncertainty quantification is only relevant within a decision framework.

This book is about applied science, not pure science. Hence, in such application there is a “utility,” or at a minimum “use-inspired” part of the scientific process of UQ. In the various applications, we saw how, ultimately, a decision is what is needed:

1. case 1: how much to re-allocate, where to drill new wells, when to stop production
2. case 2: choose between four alternative well fields
3. case 3: design of the geothermal system by deciding on the type of heat pump
4. case 4: deciding to perform acetate injection and if so, how to inject
5. case 5: deciding where to drill wells, how to complete wells

If for some reason, any UQ does not affect the decision made, simply because a deterministic model leads to a “good” decision, then no UQ is needed. It is therefore important to consider the decisions as an integral part of any UQ: otherwise, one may endlessly model to quantify uncertainty, then only to discover such exercise has negligible impact. This concept will be treated in Chapters 2 and 4 using methods of decision analysis and sensitivities involved in such decisions.

Decisions are made based on key prediction variables that are often simple quantities. Rarely are decisions made directly on complex models.

Rarely do modelers look at hundreds of complex models and decide on that basis. Key prediction variables in decision problems are often simple quantities, certainly simpler than the models on which they are based:

1. case 1: an injector efficiency (scalar), a quality map (map), a rate decline (time series)
2. case 2: recharge area (map), wetlands (rate), river (rate), contamination (map)
3. case 3: heat variation in the subsurface (space-time variable)
4. case 4: volume (scalar) and spatial distribution (map) of precipitated uranium
5. case 5: location (two parameters) or completion (about 10–20 parameters)

The fact that key prediction variables are much simpler (of lower dimension) than models (much higher dimension) can be exploited in a fit-for-purpose (sometimes also termed top-down) modeling approach. It is difficult to reduce model dimension, but it is easier to reduce dimensions in the key prediction variables. This idea will be exploited in Chapter 4 in terms of quantifying sensitivity of models and model variables on prediction variables. It will also be exploited in Chapter 7 to avoid difficult model inversion by directly focusing on the posterior distribution of key prediction variables.

Uncertainty quantification without data (and only models) is meaningless within an engineering–type, decision-making context.

Models alone cannot make accurate predictions. They can be used to understand sensitivity of model variables on prediction variables or data variables. They may provide a way to optimize data acquisition campaigns. But ultimately, if a prediction needs to be made and decisions are to be based on them, in a quantitative fashion, then field measurements are needed. The oil industry has long invested in measurements for the simple reason that they pay back tremendously in terms of management and decision making in reservoirs. The environmental sector has lagged in gathering quality measurements simply because of cost. However, if the goal is to gain a “predictive understanding” of environmental systems and to attain quantitative decision making, then gathering more data will be a prerequisite. As such, the introduction of geophysical data as presented in cases 2, 3, and 4 has gained increased attraction. Like the role of models, data are only useful if it alter decisions, not necessarily only because it inform better models or predictions. This will be treated in Chapter 2 as a “value of information” problem.

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