

8. Stochastic versus deterministic approaches

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Introduction

In broad sense, modelling refers to the process of generating a simplified representation of a real system. A suitable model must be able to explain past observations, integrate present data and predict with reasonable accuracy the response of the system to planned stresses [Carrera *et al.*, 1987]. Models have evolved together with science and nowadays modelling is an essential and inseparable part of scientific activity. In environmental sciences, models are used to guarantee suitable conditions for sustainable development and are a pillar for the design of social and industrial policies.

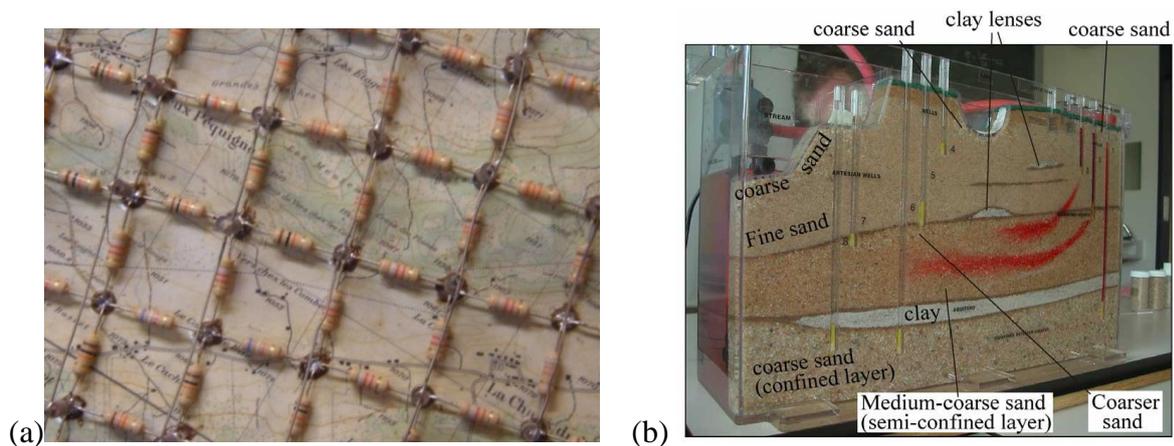


Figure 1. Types of models, (a) Electrical analog model of the groundwater flow in the Areuse catchment in Switzerland (courtesy of J.P. Tripet), (b) scale model of an aquifer [Cornaton, 2004].

Model types include analog models, scale models and mathematical models. Analog models represent the target system by another, more understandable or analysable system. These models rely on Feynman's principle [Feynman *et al.*, 1989, sec. 12-1], 'The same equations have the same solutions'. For example, the electric / hydraulic analogy (Figure 1a) establishes

the parallelism between voltage and water pressure difference or between electric current and flow rate of water. Scale models are representations of a system that is larger or smaller (most often) than the actual size of the system being modelled. Scale models (Figure 1b) are often built to analyse physical processes in the lab or to test the likely performance of a particular design at an early stage of development without incurring the full expense of a full-sized prototype. Notwithstanding the use of these types of models in other branches of science and engineering, the most popular models in environmental sciences are mathematical. A mathematical model describes a system by a set of state variables and a set of equations that establish relationships between those variables and the governing parameters. Mathematical models can be analytical or numerical. Analytical models often require many simplifications to render the equations amenable to solution. Instead, numerical models are more versatile and make use of computers to solve the equations.

Mathematical models (either analytical or numerical) can be deterministic or stochastic (from the greek 'Στόχος' for "aim" or "guess"). A deterministic model is one in which state variables are uniquely determined by parameters in the model and by sets of previous states of these variables. Therefore, deterministic models perform the same way for a given set of parameters and initial conditions and their solution is unique. Nevertheless, solving these deterministic models is sometimes difficult due to instabilities, i.e., small perturbations (often below the detection limits) of the initial conditions or the parameters governing the problem lead to large variations of the final solution [*Lorenz*, 1963]. Thus, despite the solution is unique, one can obtain solutions that are dramatically different by perturbing slightly a single governing parameter or the initial condition at a single point of the domain. Conversely, stochastic model parameters are described by random variables or distributions rather than by a single value. Correspondingly, state variables are also described by probability distributions. Thus, a

stochastic model yields a manifold of equally-likely solutions, which allow the modeller to evaluate the inherent uncertainty of the natural system being modelled.

Mathematical models (either analytical or numerical, deterministic or stochastic) can also be classified as direct or inverse. Direct or forward modelling consists of obtaining the value of the state variables given a model structure and values or distributions of the parameters governing the state equations. Instead, inverse modelling refers to the process of gathering information about the model and its parameters from measurements of what is being modeled [Carrera *et al.*, 2005]. In practice, the governing parameters and the model structure are highly uncertain. Thus, direct modeling is restricted mainly to academic purposes. On the contrary, inverse modeling corresponds to the quotidian situation, where measurements (either of parameters or state variables or both) are collected at a few selected locations in space and time and a model structure and parameter distributions are inferred from those measurements.

Either deterministic or stochastic, direct or inverse, modelling is a crucial step in environmental sciences. Just to mention one example, the disposal of nuclear wastes in deep geological formations requires the estimation of the potential environmental impact in the biosphere caused by a possible release of hazardous radionuclides. This requires detailed studies of their migration through the subsurface, including the use of numerical models to predict travel times and trajectories. A deterministic model assumes a certain geometry of the geological bodies, fractures, etc. and a deterministic (unique) spatial distribution of the parameters governing the model equations, e.g., hydraulic conductivity, storativity, etc. Thus, a deterministic model yields a unique prediction of the migration. As such, a radionuclide migrates (with probability one) to the biosphere following a 'single deterministic' trajectory and after a 'single deterministic' travel time. Unfortunately, it is impossible to get 'the perfect' characterization of geology, hydraulic conductivity, etc. because they are scarcely measured

and therefore, our knowledge is inherently uncertain. Even being omnipotent and gathering the required information at every point in space and time, the model would still be uncertain due to the presence of measurement errors. Stochastic models acknowledge model uncertainties, including (1) conceptual uncertainties, e.g., lack of knowledge about the dominant processes driving the modelled phenomena, (2) measurement uncertainties due to the limited accuracy of instruments and (3) uncertainties due to the scarcity or the lack of measurements in space and time. For instance, one can simulate the migration of the radionuclide using many different geological scenarios accounting for, e.g., presence or absence of fractures. These simulations are a set of different predictions of the migration under different conditions, from which the modeller or the policy-maker can evaluate probabilities of occurrence of a given event (e.g., probability that the radionuclide reaches the biosphere in less than 10'000 years). These events are characterized by probability distributions from which statistical moments can be evaluated such as the, minimum travel time (i.e., the maximum time for human beings to react against the migration).

Despite the aforementioned advantages, the use of stochastic models has not been excluded from debate. Stochastic models are often surrounded with an aura of esoterism and, in the end, they are often ignored by most decision-makers, who prefer a single (deterministic) solution [*Carrera and Medina, 1999; Renard, 2007*]. One might be tempted to give up and accept that stochastic processes are not amenable to the quantitative and qualitative assessment of modelling. However, it is precisely the large uncertainty associated with natural sciences that makes stochastic models necessary. The goal of this chapter is to propose a discussion of the strengths and weaknesses of deterministic and stochastic models and describe their applicability in environmental sciences. The chapter starts by outlining some background concepts and philosophical issues behind deterministic and stochastic views of nature. We then present a summary of the most widespread methods. The differences between

deterministic and stochastic modelling are illustrated by means of a real-world application in Oman. The chapter ends up with a discussion and some recommendations about the use of models in environmental sciences.

A philosophical perspective

The laws of motion exposed by [Newton, 1687] state that the future of a system of bodies can be determined uniquely, given the initial position and velocity of each body and all acting forces. This radically deterministic approach has been applied extensively to environmental problems. For example, the flux of fluids (often groundwater) through a porous medium is usually described by Darcy's law [1856] (REF) which is analogous to Ohm's law in electricity or Fourier's law in thermal energy. As most physical laws, it was first deduced from observations and later authenticated with a very large number of experiments. In groundwater hydrology, Darcy's law states that the flux of water \mathbf{q} [LT^{-1}] through a unit surface [L^2] is proportional to the gradient of hydraulic heads ' h ' (i.e., a potential, if water density is constant, that depends on water height and water pressure) and to a physical parameter k [LT^{-1}], termed hydraulic conductivity, that depends on the type of fluid and porous medium:

$$\mathbf{q} = -k \nabla h \quad (1)$$

The motion of groundwater is then described by the conservation principle, whose application leads to the very well known groundwater flow equation. It states that the mass (or the volume if the fluid is assumed incompressible) of water that enters an elementary volume of porous medium per unit time must be equal to the mass (or volume) of water that leaves that volume plus the mass (or volume) stored on the elementary volume. In terms of water volume and assuming constant density, the groundwater flow equation can be expressed as:

$$\nabla \mathbf{q} = -S_s \frac{\partial h}{\partial t} + s(\mathbf{x}) \quad (2)$$

where t [T] represents time, S_s [L⁻¹] is storativity, $\nabla \mathbf{q}$ [T⁻¹] represents the divergence of fluid flux (i.e., difference between incoming and outgoing volume of water), and r [T⁻¹] is a sink / source term that may be used to model, e.g., the recharge to the aquifer after rainfall. Note that all these parameters are, indeed, heterogeneous. Thus, they vary from one location in space to another. K and S_s can also vary in time if the aquifer changes due to changes in porosity caused by, e.g., clogging or precipitation processes. Yet, these are often considered as constant in time. Instead, recharge is a parameter that clearly depends on time. Finally, the groundwater velocity is:

$$\mathbf{v} = \frac{\mathbf{q}}{\phi} \quad (3)$$

where ϕ [-] is the effective porosity of the aquifer (i.e., ratio of the volume of interconnected pores to the total volume of the aquifer).

As one can see, this velocity can be obtained unequivocally from precise values (or spatial distributions if heterogeneity is accounted for) of the physical parameters k , S_s and ϕ , initial and boundary conditions and sink / source terms. Solving equations (1) to (3) twice with equal ingredients leads to two identical solutions, without any room for randomness. This is in line with the arguments of the German mathematician and philosopher Leibniz, who quoted the Greek philosopher Parmenides of Elea (5th century B.C.), and stated the Principle of Sufficient Reason [Leibniz, 1663-1671]: “*everything that is, has a sufficient reason for being and being as it is, and not otherwise*”. In plain words, the same conditions lead to the same consequences. This strong defence of determinism was later on smoothed by the same Leibniz

[1714], as pointed out by Look [2008]: “*most of the time these reasons cannot be known to us*”. This sentence plays a crucial role in the remainder of this section.

More than a century later, the french mathematician and physicist Laplace deeply influenced philosophy of science with his thoughts about determinism, as detailed (somewhat ironically) in his treaty of probability theory [Laplace, 1820]: “*We ought to regard the present state of the universe as the effect of its antecedent state and as the cause of the state that is to follow. An intelligence knowing all the forces acting in nature at a given instant, as well as the momentary positions of all things in the universe, would be able to comprehend in one single formula the motions of the largest bodies as well as the lightest atoms in the world, provided that its intellect were sufficiently powerful to subject all data to analysis; to it nothing would be uncertain, the future as well as the past would be present to its eyes*”. Reinterpreting the idea by Laplace, stochastics can hence be seen as a complement to deterministic modelling in the case where 'some' parameters are unknown (i.e., *epistemic* uncertainty as opposed to “*aleatory*” or “*natural*” uncertainty [Agarwal, 2008]. Following the development of statistical mechanics by Boltzman at the end of the 19th century, the rise of Planck and Bohr’s quantum physics [Bohr, 1961] has given a new legitimacy to randomness in the natural sciences during the 20th century, illustrated in the first place by Heisenberg’s famous *uncertainty principle* [Reichenbach, 1944]. Beyond epistemic uncertainty, it becomes sensible to assume that there exists an irreducible randomness in the behaviour of matter. To that Einstein replies that “*God does not play dice with the universe*” [Broglie de, 1953]. **To be clear, there is not room for uncertainty.** We prefer not to enter into this debate here, and do not distinguish what is unpredictable from what is unknown but could be predicted with more information. Coming back to the groundwater flow example, it is now clear that even with the finest mathematical and physical description of the aquifer and the best computing facilities, modellers cannot predict the groundwater flow ‘*exactly*’ unless ‘*the*’ perfect knowledge of the aquifer and its

physical parameters is available (which is, indeed, never the case in practice). Some field (or laboratory) measurements of the governing parameters are usually available and some expert knowledge is always inherited from prior studies. Thus, modellers can still use equation solvers, despite some parameters are unfortunately not known with accuracy. These have to be guessed or estimated. Plugging these estimated parameters in yields a unique solution. Yet, this solution may display a dramatic departure from reality if the parameter estimates are not accurate.

Probability theory helps to alleviate epistemic uncertainty. Instead of a single (approximated) solution, the probabilistic approach provides a manifold of equally probable solutions reflecting the many possible values (or distributions) of the unknown parameters. Of course, all but at most one of the drawn values or distributions are wrong, as is also almost surely the aforementioned deterministic estimate. Yet, the manifold of plausible solutions is not aimed at perfectly reflecting reality. Instead, it is the diversity of solutions what constitutes a richer composite information, i.e., a probability law over the set of plausible solutions. Statistical moments can then be extracted from that probabilistic law, such as the mean value (the expectation), the most frequent value (the mode), the quantification of the uncertainty associated with this expectation, (the variance) or, in a general sense, a full probability density distribution. Hence, a probabilistic model aims at capturing both the average response of the system and the variability due to uncertainties of any kind. Producing a reliable picture of this law requires some information and a suitable probabilistic representation of the underlying unknown parameters. These are respectively problems of stochastic modelling and of statistical inference:

- *Stochastic modelling* assumes that the unknown parameters have been generated by some random mechanism, and strive to mathematically characterize or partially describe this mechanism, see [de Marsily, 1994]. The latter can be achieved for

instance by assuming some parametric multivariate statistical distribution for the set of unknown parameters (in broad sense, of all input variables including, e.g., boundary and initial conditions defining the mathematical model).

- *Statistical inference* aims at *estimating* the parameters of a stochastic model on the basis of observed data. This phase, which is deeply interweaved with the chosen stochastic model and the available measurements, has inspired numerous research works of reference [*Fisher*, 1990] and is still a controversial issue nowadays [*Berger*, 1985]

In Earth Sciences, Matheron [*1989*] pointed out the difficulty of performing both a suitable model building and statistical inference based only on some observations taken from a *unique realization* of the phenomenon (assumed to be generated at random). Indeed, how could one come back to Bernouilli's law of "heads or tails" by observing the result of one single coin flipping? The same question arises when estimating the statistical law describing the spatial variability of a parameter such as, for example, the ore concentration in a gold mine. Since there is a strong dependence between neighbouring observations, the inference of a reasonable stochastic model of the ore concentration requires a sufficiently diverse sample covering the different scales at stake. The guarantee (if any) for a successful statistical inference from a unique realization of a spatial process leads to the difficult but fundamental assumption of *ergodicity* [*Matheron*, 1969]. In the same line of arguments, Matheron introduced the notion of *operatorial reconstruction* for spatial methods: in order to reach objective conclusions, the randomness attributed to a stochastic model should potentially be reconstructed from the unique observable reality.

Tools and methods

In the following, we will distinguish between (1) *statistical models*, based on statistical concepts only, (2) *deterministic models*, yielding a ‘*single best solution*’ and (3) *stochastic models*, yielding a manifold of equally likely solutions. However, the reader should bear in mind that this classification is not univocal, but just aimed at clarifying concepts. For instance, both deterministic and stochastic models make use of statistical concepts. Stochastic models are another counterexample breaking the classification. They are often formulated by a stochastic partial differential equation. Yet, they can also make use of a deterministic equation and solve it a number of times using different parameters or initial conditions drawn from a prior statistical model (i.e., a probability density function designed from available observations). This section is aimed at describing the strengths and weaknesses of these model types.

Statistical models

When a large set of field observations or measurements is available, the first step is to figure out their statistical distribution. This allows us to quantify the degree of variability of the variable under study and to investigate whether it can be summarized by a simple statistical distribution. In this perspective, the variable of interest X is modelled as a *random variable*. For example, X can be the lifetime of a radionuclide. It is well-known that not all radionuclides of the same family will decay in the same manner and exactly at the same time. Indeed, this phenomenon presents some variability. Furthermore, the fact that a radionuclide gets older does not make it more amenable to undergo decay. This phenomenon is the so-called absence of memory. Yet, despite the unpredictable nature of decay, it is still possible to define a mean lifetime of the radionuclide. This mean lifetime is the expectation $E[X]$ of the random variable X and it corresponds to its first statistical moment. Whenever it exists, the

expectation of X is defined as the sum of all possible values of the variable weighted by their corresponding probability of occurrence, or in the continuous case as:

$$E[X] = \int_{-\infty}^{+\infty} x f(x) dx, \quad (4)$$

where ‘ f ’ denotes the probability density function (pdf hereinafter) of X . Back to the radionuclide, it is not possible to calculate the theoretical expected lifetime of equation (4) if ‘ f ’ is not known (which is always the case in practice). Instead, a statistical estimation based on an available sample of observed radionuclide lifetimes $\{x_i, i \in [1, N]\}$ makes more sense.

The average, defined as:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i \quad (5)$$

is a natural estimate of $E[X]$, whose accuracy depends largely on the number of measurements N . The life expectancy $E[X]$ is however not sufficient to describe precisely the way the radionuclides decay. Since the decay may vary significantly from one radionuclide to the other, it is important to have a second statistic describing the variability of the lifetime around the expectation $E[X]$. This is what the variance (second statistical moment of the random variable X) does. The variance is defined as the expected value of the squared variation of X around $E[X]$:

$$\sigma_x^2[X] = E[(X - E[X])^2] = \int_{-\infty}^{+\infty} (x - E[X])^2 f(x) dx, \quad (6)$$

Equation (6) holds for random variables of continuous nature. Note that like in the case of $E[X]$, the x_i observations can be used as a basis to construct a statistical estimate of the variance in a discrete manner.

Overall, the expectation and the variance (most often, their estimates) play an important role in descriptive statistics. They allow us to summarize the basic properties of potentially large data sets with just two numbers. Higher order statistical moments such as the skewness and the kurtosis (third and fourth moments, respectively) are often used as well. Yet, describing a random variable with just two, three or four statistical moments is inherently limited since it does not take into account any knowledge of the physical process that generated the observed values. Estimating only the first few moments of X can therefore lead to an incomplete picture of the statistical distribution of the variable of interest. Suitable parametric models help to alleviate this problem.

In this framework, and coming back to the example, the classical approach to model the lifetime of radionuclides consists of using the following parametric exponential probability density function distribution:

$$f_{\lambda}(x) = \lambda e^{-\lambda x} \text{ for } x \geq 0, \text{ and } 0 \text{ else,} \quad (7)$$

where the positive decay coefficient (also termed rate parameter) is the unique parameter in play. When such a parametric expression is available, instead of directly estimating the mean, variance, or other moments of X , it is preferable to estimate directly the parameters controlling the distribution from the available data. In the example above, the application of integrating of the exponential distribution in equations (4) and (6) shows that $\frac{1}{\lambda}$ and $(1/\lambda)^2$ are the mean and the variance, respectively. Thus, one can use these relations to estimate $\hat{\lambda}$ from available measurements. The main advantage of this approach is that it allows, once the estimate of λ is known, to evaluate the probability of any event of practical interest. For

example, one can use the estimated pdf $f_{\hat{\lambda}}$ (equation 7) to compute the probability for a radionuclide to decay during a time interval $[a,b]$:

$$P(X \in [a,b]) = \int_a^b f_{\hat{\lambda}}(x) dx \quad (8)$$

Applications of this principle in environmental sciences are widely spread. For instance, it is very common to evaluate the probability of flood events or volcanic eruptions by first identifying a suitable parametric statistical distribution, inferring its parameters and then making forecasts (REFERENCE ?). Several difficulties may arise in this process, such as the low occurrence of extreme events in the data set. This makes the inference of an appropriate law and its parameters an arduous task (REFERENCE ?). For the sake of brevity, only the case of a single variable with corresponding pdf fully characterized by a single parameter has been described above. Still, the same concepts and methodology apply to multivariate / multiparametric problems. This method is especially useful to address the correlations between different types of observations (multivariate statistics), or between the same type of observations measured at different locations (spatial statistics).

Deterministic models

While the descriptive statistical models have the ability to capture and describe repetitive patterns observed in nature and make forecasts, they usually do not integrate physical concepts. Thus, forecasts made with those techniques might be incoherent with the underlying physics governing the process under study. For example, it is a current practice in groundwater modeling to interpolate the hydraulic head measurements $h(\mathbf{x},t)$ in space and time in a reservoir using geostatistical techniques to produce global maps [Rivest et al., 2008]. Those maps are compatible with observations and known trends. They agree with the observed spatial variability, but they are most often incompatible with basic physical

principles, such as the conservation of the mass of water in equation (2). For example, nothing guarantees that the interpolated heads in the domain would not be lower than the lowest discharge point. As such, flow directions might not make any sense. This lack of physical coherency limits the application of purely statistical methods. Instead, deterministic models are rather preferred by scientists and engineers.

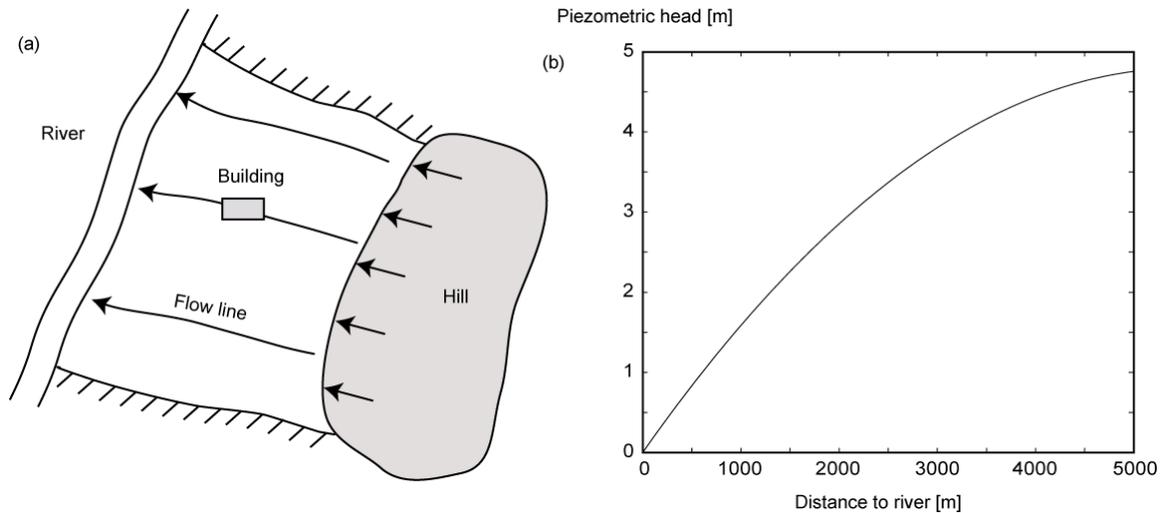


Figure 2: Example setup: (a) geometry of the problem, (b) hydraulic head distribution along a flow line computed with the deterministic solution of equation (5).

To illustrate the use of a deterministic model, let us imagine the following problem: a company is planning to build a new construction in an alluvial plain containing an aquifer (Figure 2a). The problem is then to evaluate whether the basement of the building will be below or above the groundwater table. To that end, we want to predict the hydraulic head along a flow line connecting the recharge area of the aquifer (in grey; Figure 2a) to a river that acts as a discharge area. We simplify the problem drastically to obtain an analytical solution defining the hydraulic head distribution. First, we assume that it is sufficient to consider one dimensional flow along a single flow line. In addition, we consider that the aquifer is confined (just to keep the equations amenable to didactic use), and we assume a constant recharge r due

caused by rainfall all over the domain. By combining equations (1) and (2), the simplified one dimensional problem is expressed as follows:

$$\frac{\partial}{\partial x} \left(-k \frac{\partial h}{\partial x} \right) = p \quad (3)$$

This partial differential equation is one typical expression of a deterministic physical model used in groundwater hydrology. As explained above, it was derived from the conservation principle and a phenomenological law (Darcy's law). It was expressed for a given geometry and with several simplifying assumptions (compressible fluid, steady-state, etc). Solving a for unique solution of equation (3) requires some boundary conditions. In this example, we assume that the hydraulic head is equal to a given value h_r along the river located at $x=0$ (actually, h_r is the elevation of the water table at the river), and that the flux entering the aquifer along the foothill ($x=L$) is equal to q . The integration of equation (3) using the aforementioned boundary conditions yields the following unique solution:

$$h(x) = \int_{u=0}^{u=x} \frac{p(L-u)+r}{k(u)} du + h_r. \quad (4)$$

If, in addition one assumes the hydraulic conductivity k constant in space, we get:

$$h(x) = -\frac{p}{2k} x^2 + \left(\frac{r+pL}{k} \right) x + h_r. \quad (5)$$

which expresses how the hydraulic head varies within the domain for any values of the parameters describing the geometry and properties of the aquifer. For a given set of parameters, the solution to equation (5) can be calculated and plotted. Figure 2b displays the solution obtained with $k=10^{-2}$ m/s, $r=100$ mm/year, $q=5$ m/year, $L=5$ km. Unfortunately, such type of analytical expressions cannot be obtained in practice, either because the geometry is too complex or because the parameters vary in a complex manner (e.g., hydraulic conductivity changes depending on the geological material or precipitation and recharge vary

in space and time). Therefore, deterministic models are usually solved with numerical techniques such as finite elements or finite volumes [Huyakorn and Pinder, 1983]. Overall, the main strength of the deterministic approach is that it allows us to understand the influence of certain parameters or processes on the variables of interest. It also allows us to make forecasts based on well established physical principles. In practice, we have seen that those forecasts can either be obtained via simple analytical expressions such as equation (5) or, more generally, by solving complex numerical models, which is often the case in practice.

Stochastic models

The limitation of deterministic models is that they do not account for uncertainty. The parameters governing the equations are supposed to be known and the solutions are therefore unique. This often poses a practical problem because nature is intrinsically heterogeneous and the system is only measured at a discrete (and often small) number of locations. Therefore, even if the physics of the system is relatively simple and understandable by deterministic equations, it is difficult to trust the solutions of deterministic models because the input parameters, model geometry, initial and boundary conditions, etc. are not well known or, in best case, never known exhaustively. Still, it would also be a waste not to take into account the physics. Stochastic methods can be regarded as a tool to combine physics, statistics and uncertainty within a coherent theoretical framework. On the one hand, the unknown parameters are described by statistical distributions. On the other hand, the different variables describing the problem are related to each other and to the (uncertain) model parameters through (deterministic) physical laws. The resulting models take the form of stochastic partial differential equations.

Coming back to the simple groundwater example, the recharge r and the inflow q may not be known accurately. Consequently, these two parameters can be viewed as random functions

that vary in space and/or time but that have some statistical properties (such as a mean, covariance, etc.) that can be inferred from samples. Considering them as random functions implies that the hydraulic head h is also a random function, related to r and q through equation (3) and the corresponding boundary conditions. In that case, equation (3) is interpreted as a stochastic differential equation because it relates random functions and not simply spatio-temporal functions. Under certain simplifying assumptions, one can derive also analytically the statistics of the random function h . For example, if we assume that k is known and constant in space (despite both assumptions are, indeed, aberrant), equation (5) holds and the expected value $E(h)$ of the hydraulic head can be expressed as:

$$E[h(x)] = E \left[-\frac{p}{2k} x^2 + \left(\frac{r+pl}{k} \right) x + h_r \right] = -\frac{E[p]}{2k} x^2 + \left(\frac{E[r]+E[p]L}{k} \right) x + h_r \quad (6)$$

This simple equation states that we can directly estimate the expected value of the hydraulic head at any point of the domain $E[h(x)]$ if the expected values of recharge $E[r]$ and inflow $E[q]$ are known. Note that equations (5) and (6) are identical but for the fact that the meaning of the intervening parameters has changed, i.e., the deterministic values of r and q have been replaced by their expected values. Following the same logic, one can compute the variance of the hydraulic head at any point in the domain:

$$\sigma_{h(x)}^2 = \left[\left(L - \frac{x}{2} \right)^2 \sigma_p^2 + \sigma_r^2 + \left(L - \frac{x}{2} \right) \text{cov}(p, r) \right] \left(\frac{x}{k} \right)^2 \quad (7)$$

This interesting expression shows that the variance is zero (i.e., no room for uncertainty) at the vicinity of the river ($x=0$). This makes sense because the boundary condition there states that the hydraulic head in the aquifer is equal to the water elevation in the river h_r . Thus, there is no uncertainty regardless of those of uncertain parameters (unless the boundary condition h_r is also considered as a random function). As expected, the uncertainty increases with distance to the river. This approach allows us to plot the uncertainty bounds corresponding to the

expected value plus / minus two times the standard deviation (Figure 3a). These are the so-called 95% confidence intervals.

Alternatively, one can address the uncertainty by applying the deterministic solution in equation (5) using extreme values of the unknown parameters p and r . To that end, we assume that the only uncertain parameter is now recharge and that it can be represented by a Gaussian distribution with known mean (100 mm/year, the deterministic value used before) and standard deviation (i.e., the square root of the variance, 10 mm/year in this case). Under such assumption, recharge values lie in the corresponding 95% confidence [80, 120] mm/year. Solving the deterministic equation in (5) with these two extreme values yields two solutions for the hydraulic head that depict an envelope of possible values of h (Figure 3a, red lines). However, this is not a good option because this envelope defining the uncertainty is much larger than the one defined by the stochastic model (Figure 3a, green lines). This difference increases with the variance of the unknown parameter. Another argument to defend the use of stochastic models lies in the fact that the stochastic formulation of the problem allows us to obtain the full range distribution of hydraulic head (i.e., the complete pdf) that accounts for possible correlations between the different sources of uncertainty (Figure 3b).

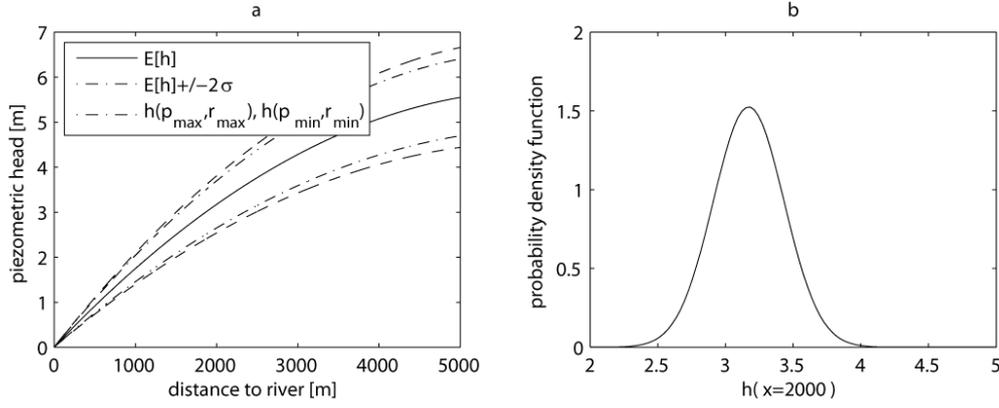


Figure 3: (a) Comparison between uncertainties obtained by deterministic and stochastic models. Recharge is the only uncertain parameter. In black, expected head distribution along the flow line obtained by the stochastic model (visually comparable to that in Figure 2b, output of the deterministic model). The uncertainty is estimated either using the stochastic approach of equation (7) (green lines), or using a min/max deterministic approach (red lines); (b) probability density function of hydraulic head at the location of the building obtained by using equation (7) and the assumption of Gaussian uncertainty.

In most cases it is not possible to derive simple expressions such as equations (6) and (7). Several alternative methods exist to obtain exact or approximate statistical relations between the variables and the parameters governing a stochastic partial differential equation. In broad sense, these methods consist of obtaining expressions for the first statistical moments of the variable of interest and relating them to the moments of the input variables. Under certain circumstances, it is possible to obtain directly the expression of the pdf of the variable of interest. This is used for example in fluid mechanics for turbulent flow [Jenny *et al.*, 2001] but, most generally, approximate expressions are derived either through small perturbation analysis, in which the variables are decomposed as a mean plus a perturbation around it. By construction, this perturbation has a zero mean, and a variance equal to the variance of the original variable. Plugging these definitions into the deterministic equation, one obtains an equation that is then decomposed into sub-equations of same order. To solve it, one can

neglect terms that are considered of small order and obtain approximate solutions. A simple illustrative example can be found in [de Marsily, 1989]. In the field of groundwater, one can find a detailed description of those techniques as well as a recent overview of the main results in the books by Zhang [2002] or Rubin [2003].

However, the limitation of the perturbation approach and other approximate techniques is that their results are valid only for small variances. In addition, the results are usually expressed in terms of mean, variance and covariance even if the distribution is known to be non multi-Gaussian (e.g., the variance does not need to be bounded). To overcome these limitations, the most general approach is the Monte Carlo method [Metropolis and Ulam, 1949]. It generates a series of samples from the statistical distribution of the input parameters and solves the deterministic equations (either analytically or numerically) for each set of parameters. One then obtains an ensemble of responses for the variable of interest. Repeating the operation a large number of times (i.e., sampling the space of parameters exhaustively) allows us to infer the statistics of the variable of interest.

To illustrate how this method works and to demonstrate the importance of such analysis, we will consider again the groundwater problem of Figure 2. Yet, this time we will consider that the hydraulic conductivity varies in space and, indeed, that it is not known everywhere in the domain. We will assume just that the hydraulic conductivity follows a log-normal distribution with known mean $k=10^{-2}$ m/s and variance $\sigma_{\ln(k)}^2 = 1$. This might seem a strong assumption.

However, gaussianity is often supported by field data (or a suitable transform of them, as logarithmic in this case). We will also assume that the log-hydraulic conductivity field can be modelled by a multi-Gaussian spatially correlated field having an exponential covariance function with a correlation range of 200m. Figure 4a displays an example of a correlated random field generated with those parameters. The hydraulic conductivity is centered on the

value used previously in the deterministic model ($k=10^{-2}$ m/s) and varies within an order of magnitude around this mean value. This field is not conditioned to any local data. We have generated 2000 hydraulic conductivity fields for the Monte Carlo analysis. They all look similar but vary in a random manner around the mean with structures that always display the same pattern type and size. For each field, equation (4) is solved numerically by integrating the hydraulic head along the flow line. This provides 2000 equally-likely distributions. Two of them are depicted in blue in Figure 3c. These are comparable with the deterministic analytical solution depicted in red in Figure 2b. The first observation that becomes apparent from Figure 3c is the effect of the heterogeneity of k , translated into local variations of the slope of the blue curves. The ensemble of the 2000 simulated head distributions is the main result of the Monte Carlo analysis (Figures 2b and 2c in green). One can observe there that the local fluctuations of h have been smoothed out due to the averaging. This effect is caused by the large number of simulations carried out and would diminish if the size of the ensemble would decrease.

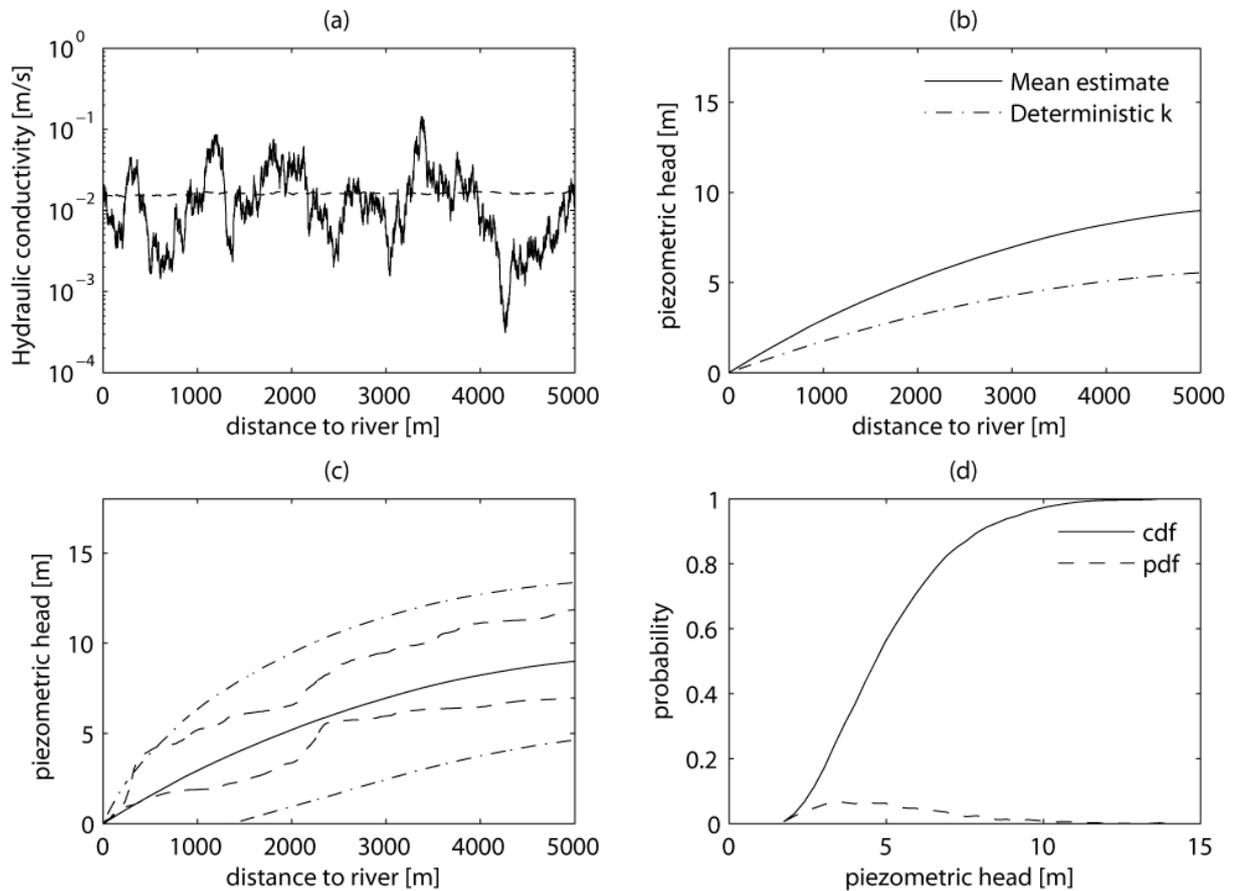


Figure 3: Monte Carlo analysis of the problem illustrated in Figure 2 when the hydraulic conductivity k is the unique source of uncertainty. (a) example of a random hydraulic conductivity field, (b) comparison between the mean hydraulic head of 2000 Monte Carlo simulations (in green) and the deterministic head distribution obtained with a constant mean deterministic k (red line), (c) results of the Monte Carlo procedure: mean hydraulic head as a function of x (in green), two individual simulations of h (in blue), and the envelope of the 95% confidence interval (dash-dotted lines), (d) probability density distribution (dashed line) and cumulative probability density distribution (solid line) of the hydraulic head at the location of the building ($x=2000\text{m}$).

In practice, one is often not interested in the results of the simulations separately, but in the statistics of the ensemble of all the simulations together. The first thing that can be done is to calculate the statistical moments of the ensemble, such as mean and variance, and plot them as

a function of space (and / or time, if necessary). This is displayed in Figure 3c where the green line depicts the ensemble average (mean) of all simulated hydraulic head distributions as a function of the distance to the river. Dashed-dotted lines depict the mean plus or minus twice the standard deviation of the numerical results (i.e., the 95% confidence interval). This allows us to see rapidly the envelope in which most of the simulations fall (more than 95% if the distribution is Gaussian). Thus, this is a clear illustration of the amount of uncertainty on the hydraulic head at any location in the domain. In plain words, the larger is the envelope, the larger is the uncertainty of the solution. A very important result arising from Monte Carlo analysis is that the mean hydraulic head (the same can be made for the median or the mode) can be significantly different from the hydraulic head computed with the same deterministic model using the mean value of the hydraulic conductivity, assumed to be constant in space (Figure 2b). One can observe that the mean hydraulic head is about two times higher than the value computed by the deterministic model. Another way to look at the same results is to analyze the probability distribution of hydraulic head at a location of interest. For example, the hydraulic head at the future location of the building ($x=2000$). The deterministic model assuming a mean and constant hydraulic conductivity (equation 5) estimated at that location a single hydraulic head value of 3.17m. Instead, the Monte Carlo approach allows us to compute the histogram of all possible values at that location. From that histogram, the cumulative density function and / or the probability density function can be estimated (Figure 3d). The distribution is not symmetric, as revealed by its third statistical moment (skewness=??), it has a median equal to 4.7m, significantly larger than the deterministic estimate (3.17m) and displays a wide range of possible values between 1.6m and 15m. The manager of the construction can use both types of results for risk analysis. In terms of design for the construction project this opens the way for two approaches. On the one hand, the manager can include the uncertainty results in the design of an optimal construction scheme

using, e.g., loss function analysis [Srivastava, 1990] to take the decision that will minimize the expected financial losses. On the other hand, when the uncertainty is large and, consequently, the risks too high, the manager can decide to gather additional data to reduce the uncertainty. Again, the stochastic model can help to locate those additional measurement points.

As compared to the deterministic method described earlier, the advantage of the Monte Carlo approach is that it can be applied for any statistical distributions (including non parametric distributions) and make use of any deterministic model. In particular, the deterministic model can be very complex and does not need to be linear. This is the main reason why this approach has been used extensively in a wide manifold of applications [Naff *et al.*, 1998; Sambridge and Mosegard, 2002]. The limit of the Monte Carlo approach is that it may be extremely time consuming when complex deterministic (numerical) models need to be computed many times (e.g., three dimensional, non-linear transient, etc.).

A practical illustration in Oman

This section illustrates the concepts of deterministic and stochastic modeling introduced previously. To that end, we use real data gathered in a coastal aquifer in Sur (Oman), where a desalination facility currently pumps brackish groundwater at an insufficient rate to satisfy the growing demand of freshwater in the area. The aim of this work was to design a new pumping network to increase the current extraction roughly by a factor of 9 [Alcolea *et al.*, 2009]. To that end, new pumping wells needed to be sited and their pumping rates defined. The aim was to achieve the target discharge while minimizing the environmental side effects (i.e., minimum drop of the hydraulic head) and the demand of energy for the pumping, thus minimizing the total cost of the solution.

In that study, the main source of uncertainty was on the geology of the coastal aquifer. This is made of karstic limestone with interbedded conglomerates on top of a marl deposit. The marine environment causes partial dissolution of the limestone by interaction with seawater. Consequently, the host rock presents karstic cavities as well as a large number of irregularly distributed small conduits. The hydraulic conductivity is very high at those karstic features while it drops dramatically at places where no dissolution occurred. The location of these karstic features is, indeed, not known a priori.

The work consisted of two main steps. First, the aquifer was characterized using a stochastic approach. The resulting model describes the system in the absence of the target pumping network. Second, once the model properly represents the expected patterns of aquifer heterogeneity and architecture (i.e., when the model is properly inversely calibrated and honors available data), it is used to forecast the impact of pumping at the new potential wells and to define the optimum pumping scheme.

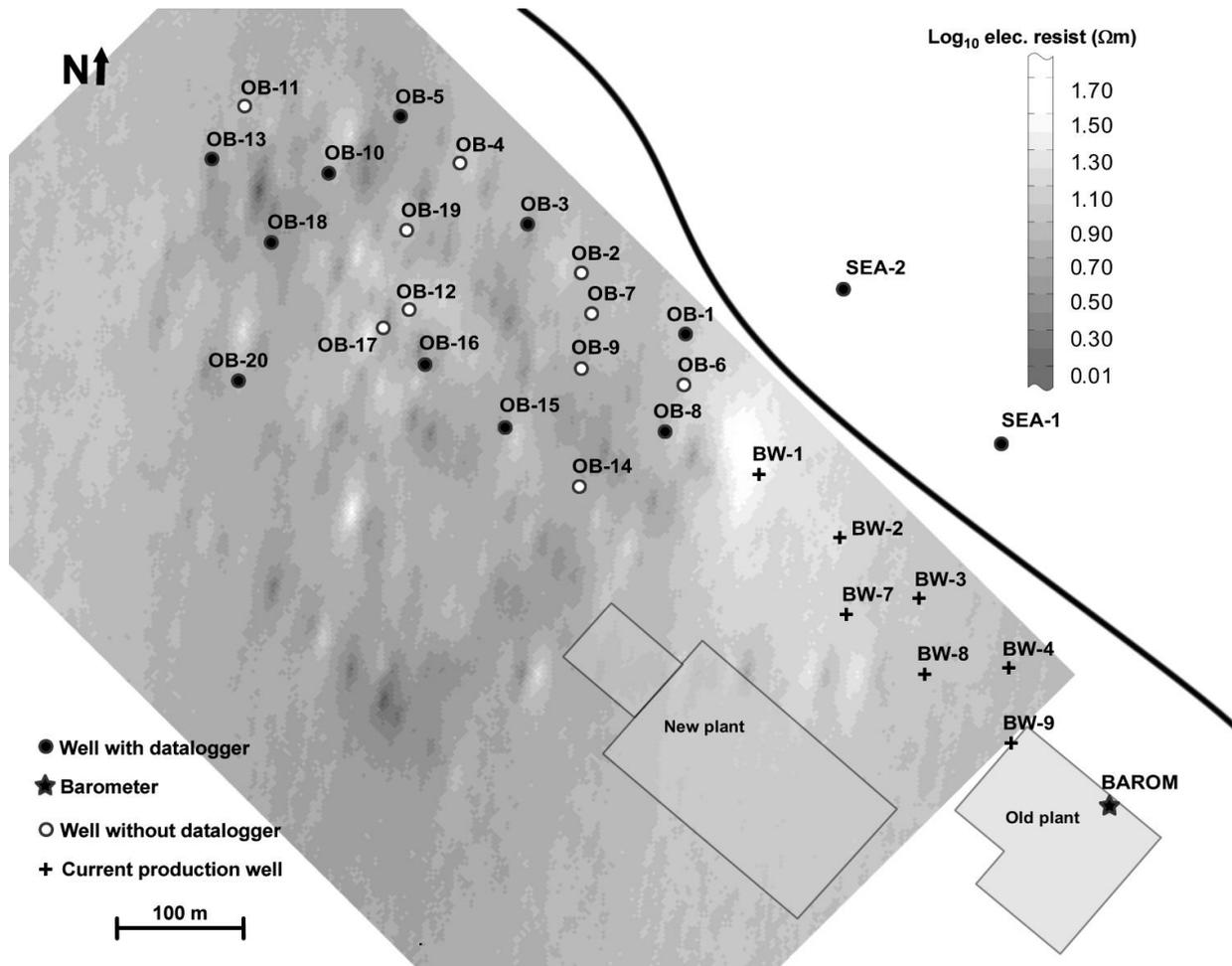


Figure 4: Map displaying the location of the observation boreholes (OB) and current production beach wells (BW). The hydraulic head at observation wells depicted by black dots was continuously monitored. Two sensors (SEA-1 and SEA-2) were located at the sea-shore for measuring the sea level fluctuation. A barometer (depicted by a star) was located at the old desalination plant. The background image depicts the estimated electrical resistivity arising from a preliminary geophysical campaign. From Alcolea et al [2009].

The construction of the model followed 3 main steps. First, hydraulic conductivity measurements arising from three pumping tests and geophysical data (Figure 4) were used to build a geostatistical model of the hydraulic conductivity field $k(x,y)$. More precisely, the field was assumed to be multi-Gaussian and to follow a lognormal univariate distribution. Therefore its inference requires the definition of just its mean and covariance from available

field data. In addition, a transient deterministic finite element model representing the groundwater flow towards the sea was built. This model allows us to calculate the hydraulic head distribution as a function of space and time $h(x,y,t)$ for a given hydraulic conductivity field $k(x,y)$. Generating many k fields and solving the deterministic model with them allows us to estimate the uncertainty on hydraulic head as described in the previous section.

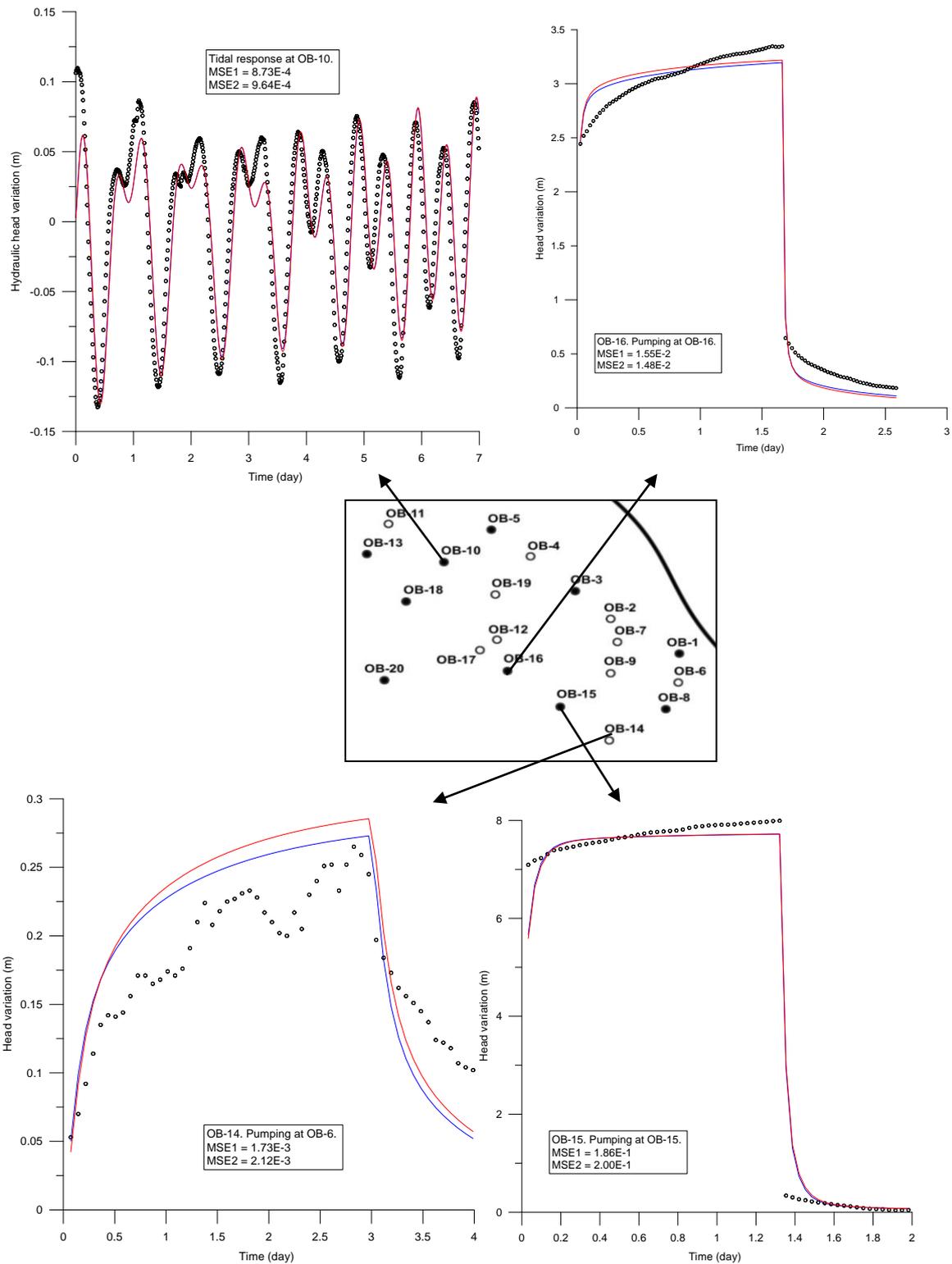


Figure 5: Calculated and measured head variations at selected points in response to tidal and pumping effects. Hydraulic heads from two simulations are depicted in red and blue. Measurements are depicted with circles. In the insets, MSE denotes mean square error (mean square difference between calculated and measured head variations).

However, based on this first model only, the uncertainty would be unrealistically large. Therefore, it is important to constrain the stochastic model with the available temporal series of hydraulic heads. Indeed, these vary in space and time (Figure 5) in response to tidal fluctuations along the northernmost boundary of the aquifer and in response to the three large scale pumping tests conducted in the aquifer for this study. The recorded signal of hydraulic head variations measured at available observation wells contains indirect information on the spatial distribution of hydraulic conductivity. Constraining it in such a way that the calculated heads are similar to the observed heads is a typical inverse problem amenable to be solved in a stochastic framework. This inverse problem can be solved using different techniques in the framework of multi-Gaussian fields [*Carrera et al.*, 2005; *de Marsily et al.*, 1999; *Hendricks Franssen et al.*, 2009]. Here, the Regularized Pilot Points Method [*Alcolea et al.*, 2006] was used to obtain 200 Monte Carlo simulations of the hydraulic conductivity and storativity fields (not displayed here) constrained by all available data. Four of these simulations are depicted in Figure 6.

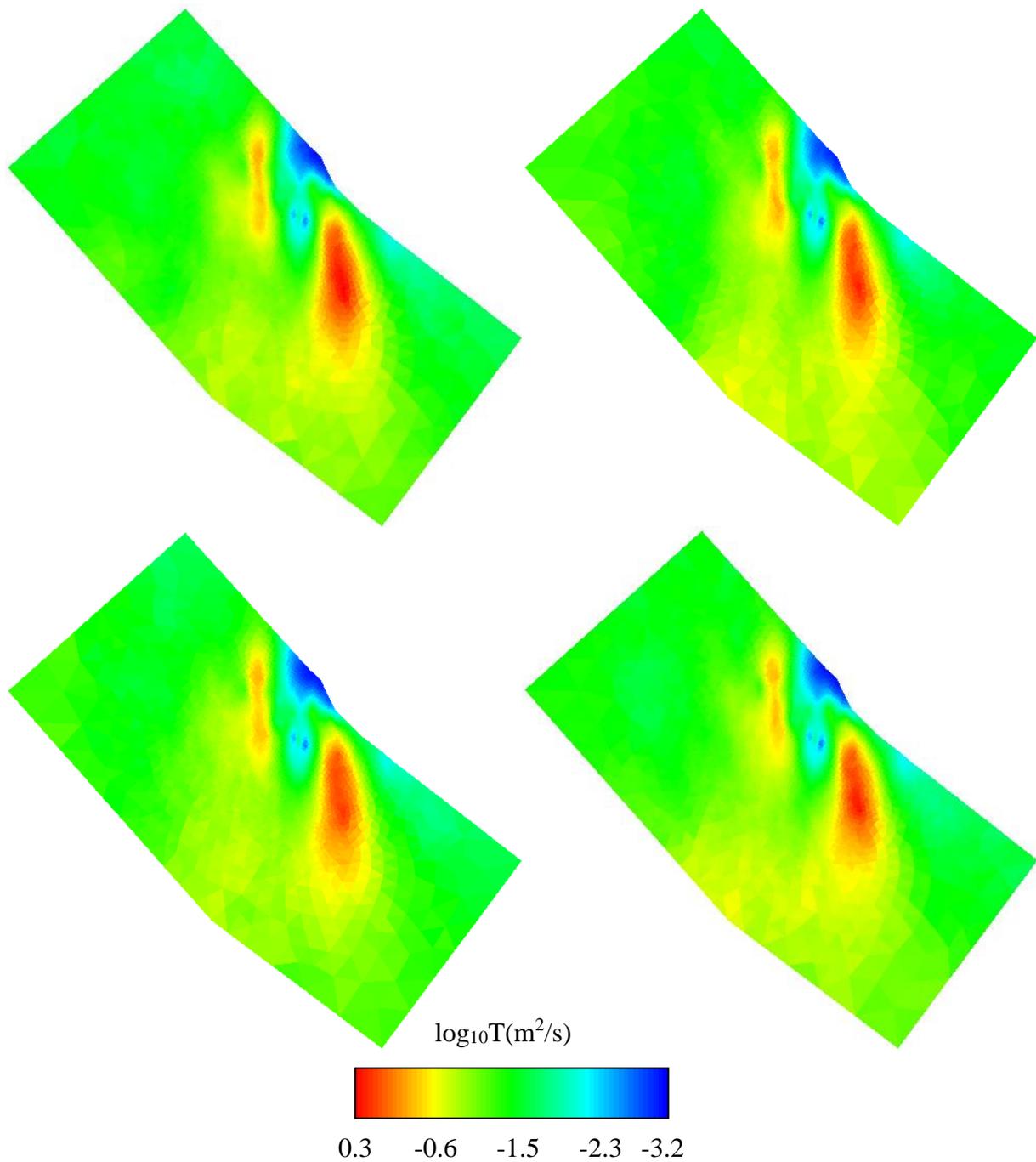


Figure 6: Four out of two hundred Monte Carlo simulations of the stochastic transmissivity field (i.e., integral of hydraulic conductivity along a vertical profile) conditioned to transmissivity data and available hydraulic head temporal series.

The goodness of these characterizations is evaluated in terms of fits to available head data (Figure 5) and physical plausibility of the inverted hydraulic conductivity and storativity fields. The latter is evaluated visually (Figure 6). All the aforementioned simulations present highly conductive channels (possibly karstic conduits), well connected to the sea. This corresponds to the initial guess (i.e., karstification caused by dissolution). They also reveal zones with very low hydraulic conductivity close to the seashore. This can be explained by the deposition of fine, less permeable, materials along the coast line. Fits to available head data are displayed in Figure 5. They are in all cases satisfactory.

The hydraulic conductivity fields were then used to define the optimal locations and corresponding production rates of the pumping wells. To that end, we made use of a genetic algorithm minimizing a penalty function accounting for the operational and maintenance costs. One particular aspect of the optimization when dealing with stochastic models is that many different and equiprobable descriptions of the reality are considered. For each description, a different pumping network configuration is optimal. But only one single pumping scheme will be implemented in the field. Therefore the optimum solution must be defined over the ensemble of the possible Monte Carlo simulations using a criterion of robustness: the optimum design should be efficient for all of them. It may not be the optimum if we would know the real distribution of hydraulic conductivities but it should never be a bad solution whatever the reality is (if the number of simulations is large enough, as in this case). Applying those principles, the optimum pumping network was obtained (Figure 7a). For illustration purposes, we compare its performance with the one of a deterministic, tradition-based, hand delineated, pumping scheme configuration (Figure 7b).

In broad terms, the most important benefit of the stochastic approach described above was to allow us to estimate at any stage of the study the remaining uncertainties and therefore the risks that could be evaluated by decision and policy makers. This was used at a first stage to

estimate the feasibility (both technical and economical) of the project and later to design the optimum pumping scheme. At the end of this last stage, uncertainty was still remaining. This effect will be omnipresent because any new simulation of the hydraulic conductivity field will add information to the ensemble and, therefore, a new bunch of possibilities with regard to the design of the pumping network. This uncertainty is depicted by the cumulative probability density distribution of the cost of production and of the hydraulic head drop at the pumping wells (Figures 7c and 7d). There, one can also compare the performance of optimum and tradition-based deterministic pumping schemes. The optimum distribution of wells (and corresponding flow rates) is reasonable, as observed in Figure 10. In general, largest pumping rates are located at the highly conductive bodies. This causes small hydraulic head drops and a superior yield of the pumping scheme. In addition, the total cost is reduced substantially (about 10% of the total cost). Based on those graphs, the decision maker can have a pretty good idea of the investment required to run the project and the corresponding uncertainties and risks. Similarly, the uncertainty on the environmental impact of the project is evaluated in a stochastic manner for the two scenarios in Figure 7d.

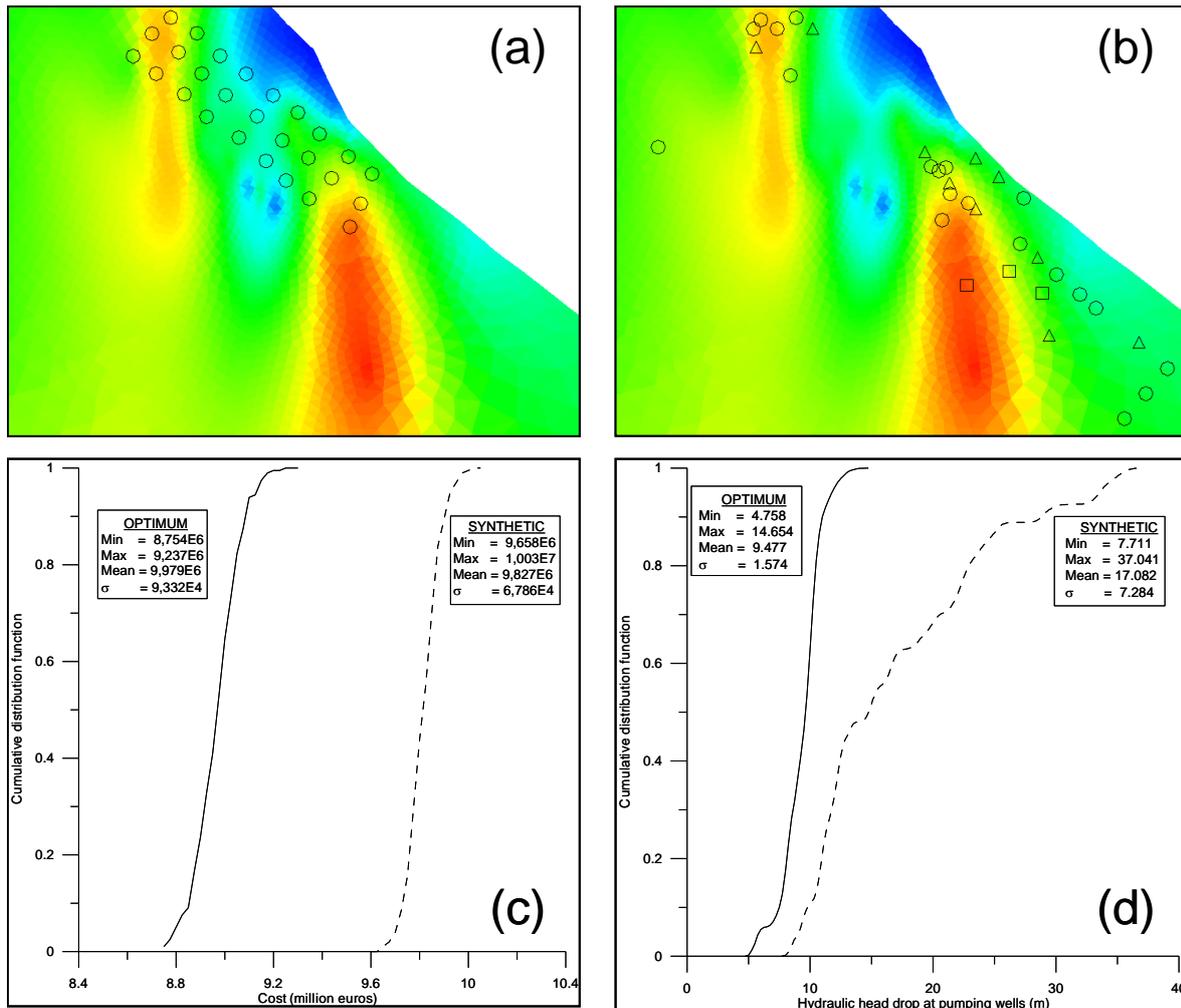


Figure 7: Synthetic (a) and optimum (b) pumping networks. Pumping rates of 100 l/s, 70 l/s and 30 l/s are depicted with circles, triangles and squares, respectively. On the background, the average transmissivity field plotted with the same scale as in Figure 6. Cumulative distribution functions of optimum (solid line) and synthetic (dashed line) pumping networks: (a) cost function, (b) hydraulic head drop at pumping wells.

Discussion

At least three main types of mathematical models are used in environmental sciences: (1) statistical models that allow us to summarize the main patterns of variability using statistical concepts only, (2) deterministic models yielding a ‘unique best’ solution based on well established physical laws and principles, and (3) stochastic models yielding an ensemble of equally-likely solutions of the phenomenon under study, which can be seen as a combination of a statistical and deterministic models. This classification is by no means univocal. Yet, it is useful to illustrate the strengths and weaknesses of the different modeling strategies analyzed in this chapter.

As pointed out by Prigogine [*Prigogine, 1997*], these model types have been traditionally rivals. We argue, first, that these views of nature are complementary. Second, these model types are more and more applied nowadays in synergy rather than in competition, i.e., the three of them can be used at different stages of the same project. More interesting, complex patterns at a small scale are often difficult to model using a deterministic approach because the number of unknown parameters intervening in the characterization is too large. One can, for example, consider the behavior of individual molecules in a gas and their interactions. Changing the scale of observation to a macroscopic one (upscaling) and introducing macrovariables such as temperature (that can be easily defined using a statistical approach), one can infer some new deterministic physical laws that allow us to understand the global behavior of the system without describing the internal (molecule to molecule) complexity. In that upscaling process, we see through the use of stochastic methods the emergence of different levels of deterministic laws. A second example that has been used here to illustrate different concepts is groundwater flow. This can be described by the Navier-Stokes equations if the three dimensional geometry of the pore network is known and if one can discretize the

pore space finely. That approach is indeed limited to very small samples of material (a few mm³) to be amenable to solution with existing computers. Yet, one can define expected values for the pressure (or hydraulic head) and the fluid velocities and derive analytical expressions for the mean behavior of the fluid on a larger domain. Doing so, one can obtain Darcy's law from the small scale equations [*de Marsily*, 1989].

Because of all those reasons, we believe that the traditional (and controversial) question on the choice of a statistical, deterministic or stochastic approach to model environmental processes is obsolete. The world should not be considered as a summary of statistical moments (statistical models), neither perfectly known (deterministic) nor perfectly random (stochastic). The three views of nature need to be used altogether and need to be integrated. Certainly, this requires an additional effort from scientists and engineers who have to become familiar with the three approaches. Still, we argue that there is no way nowadays to make the economy of one or the other type of models. Indeed, no one can reasonably argue that a single characterization of a natural system is sufficient to represent our current understanding. Neither does it make more sense to argue that everything is known with 100% accuracy than to argue that physical laws are irrelevant.

To conclude, it is therefore necessary to highlight that the set of methods discussed above are extremely efficient to describe regularities and produce forecasts based on the underlying assumptions that we observed in the past has a high chance to be reproduced in the future, or that the observations made on a region of the earth have also a good chance to be applicable in another location. This is how we can infer statistical models, derive physical laws and build theories and models. That type of reasoning is generally true and has allowed mankind to make enormous progress. But this is not always true and this is where the limits of these approaches lie. When extreme events are not present in the data sets and in the observations, there is almost no way to predict them with reasonable accuracy. When the conceptual models

on which the deterministic models are based do not include some crucial features that have not been observed, there is very little chance that the forecasts will be correct, and there is little chance that the stochastic models will include such exceptional features. Therefore, the modeler must always remain very humble and remind that the probability estimates, even if they were derived with a very rigorous mathematical treatment, are only based on a subsample of the real events. This argument is sometimes used to defend the idea that stochastic methods are not useful and that mini-max or scenario analysis are much more reasonable. Our vision is that the choice of a model must be based on the needs and constraints for a given project, as well as on the current level of knowledge and resources. The choice must not be dogmatic but driven by the principle of maximum efficiency to solve a given problem.

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