

Chapter 1

Introduction

The German physicist Werner Heisenberg once said, “What we observe is not nature herself, but nature exposed to our method of questioning.” Mathematical models have long served as such a tool of questioning. A mathematical model of a physical system quantitatively describes the relationship among various variables that characterize the states, internal structure, and external conditions of the system.

In Sect. 1.1, several commonly seen models in environmental and water resources (EWR) studies are shown. A general form of mathematical models and their classifications is then provided. Different mathematical models are constructed across different science and engineering disciplines. Models used in the EWR fields are often nonlinear, dynamic, stochastic, and governed by partial differential equations (PDEs). The traditional process of constructing a EWR model involves data collection, conceptualization, model calibration/parameter estimation, and finally, the evaluation of model reliability. During this process, the following problems must be solved: (1) the *forward problem* for simulation and prediction; (2) the *inverse problem* for model calibration and parameter estimation; (3) the *design problem* for effective data collection; and (4) the *reliability problem* for model application.

In EWR modeling, the solution of forward problem has become routine. We assume that readers of this book are already familiar with the solution of forward problems in their own fields. Thus, no attempt is made to survey numerous forward solution techniques existing in the literature; instead, a brief introduction to basic analytical and numerical methods is provided in Sect. 1.2.

Data types available for model construction include prior information, direct measurements of parameters, observations of state variables, as well as the accuracy requirement of model applications. Depending on the availability and use of different types of data, different approaches and criteria for model calibration and parameter identification exist. The *classical inverse problem* (CIP) reverses the forward solution to seek model inputs from model outputs, under the assumption that the model structure error is absent. In Sect. 1.3, two common criteria, “fitting observed data” and “using prior information,” are used to formulate the inverse problem in both deterministic and statistical frameworks. The *extended inverse problem* (EIP),

requiring the identification of both model structure and model parameters in an adaptive sense, is also introduced in that section.

The model reliability problem to be introduced in Sect. 1.4 has recently become one of the most concerned issues in EWR modeling. But this problem is very challenging because of the inherent difficulties related to determining the model scale, model complexity, and data sufficiency. The *goal-oriented inverse problem* (GIP) incorporates “reliability assurance” as the third criterion in its formulation, in which separate models are constructed for the same system according to the goals of model applications and associated accuracy requirements.

1.1 Mathematical Modeling

1.1.1 Modeling an Open System

A EWR system, such as a watershed or groundwater basin, is an *open system* that continuously exchanges mass and/or energy with its surroundings. The states of a EWR system are determined by both its internal structure and external conditions. The following types of variables are often used to characterize a EWR system:

- *State variables* that characterize the states of a system
- *System parameters* that characterize the structure and properties of a system
- *Boundary parameters* that describe the outer conditions of a system in both spatial and temporal domains
- *Control variables* that represent external forces acting on a system.

Mathematical models are omnipresent in EWR fields, including surface hydrology, hydrogeology, environmental engineering, petroleum engineering, agriculture, ecology, and cross-disciplinary fields coupling two or more of these individual subjects. These EWR models are derived from the laws of mass, energy, and momentum conservation, empirical formulas, constitutive relationships, or statistical learning theory. They are also determined by appropriate subsidiary conditions and assumptions used during model simplification. Some examples are given below.

1.1.2 Examples of EWR Models

Example 1.1 *The Monod model of biomass growth*

Monod model is used for describing the growth of microorganisms (Bungay 1998)

$$\mu = \frac{\mu_{\max} S}{K_s + S}, \quad (1.1.1)$$

where μ is the specific growth rate, S is the nutrient concentration, μ_{\max} is the maximum specific growth rate, and K_s is the Monod coefficient. In this model, μ is the state variable, S is the control variable, and μ_{\max} and K_s are model parameters to be determined by experiments. In (1.1.1), the state variable is given explicitly by an algebraic equation.

Example 1.2 *A convolution integral model for spring discharge prediction*

The relationship between precipitation rate $p(t)$ and spring discharge $q(t)$ in a basin can be represented by the following model (Beven 2001)

$$q(t) = \int_0^t K(t - \tau) p(\tau) d\tau, \quad (1.1.2)$$

where the transfer function $K(\cdot)$ reflects catchment characteristics and can be obtained from historical observations of $p(t)$ and $q(t)$. In this model, $K(\cdot)$ is the model parameter, $p(t)$ is the control variable, and the state variable $q(t)$ is given by a convolution integral.

Example 1.3 *Lumped parameter rainfall–runoff model*

A lumped parameter rainfall–runoff model of a watershed can be expressed in the following general form (Sorooshian 2008; Beven 2001)

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}, \boldsymbol{\theta}, \mathbf{p}), \quad (1.1.3)$$

where the watershed is divided into M subbasins, $\mathbf{u} = (u_1, \dots, u_M)^T$ is the state vector, with its i th component representing the average soil moisture content of the i th subbasin, $\mathbf{f}(\cdot)$ is a nonlinear operator representing the system transition over an instant of time, $\boldsymbol{\theta}$ is a set of system parameters, and $\mathbf{p}(t)$ is a forcing term whose i th component represents the average precipitation rate over the i th subbasin. Equation (1.1.3) is a set of ordinary differential equations (ODE), and an appropriate initial condition $\mathbf{u}(t)|_{t=0} = \mathbf{u}_0$ is needed for its solution. It can be considered as a discretized form of a distributed parameter rainfall–runoff model.

Example 1.4 *Channel flow model*

Water flow in a shallow river can be modeled by the Saint Venant equations, which assume 1-D flow, small bed slopes, and hydrostatic pressure distribution in the vertical direction (Chow 1959)

$$\frac{\partial h}{\partial t} + \frac{\partial(hv)}{\partial x} = q \quad (1.1.4)$$

and

$$\frac{\partial v}{\partial t} + g \frac{\partial h}{\partial x} + v \frac{\partial v}{\partial x} = F(v, h). \quad (1.1.5)$$

In (1.1.4), x is the longitudinal distance along the river, $h(x, t)$ is the water depth, $v(x, t)$ is the flow velocity, and $q(x, t)$ denotes the lateral inflow rate per unit length of the river. In (1.1.5), g is the acceleration of gravity; $F(v, h) = S_0 - S_f$, where S_0 is the riverbed slope, S_f is the energy slope defined as $v^2 / c^2 h$, and c is a roughness coefficient. The 1-D Saint Venant equations are nonlinear first-order PDEs that require appropriate auxiliary conditions to solve for $h(x, t)$ and $v(x, t)$.

The appropriate auxiliary conditions for (1.1.4) and (1.1.5) include initial conditions $h(x, 0) = f_0(x)$ and $v(x, 0) = g_0(x)$ at $t = 0$ and boundary conditions $h(0, t) = f_1(t)$ and $v(0, t) = g_1(t)$ at the upstream end $x = 0$, where f_0, f_1, g_0 , and g_1 are known functions. This model consists of two coupled nonlinear PDEs with the state variables $h(x, t)$ and $v(x, t)$, control variable q , parameters c and S_0 , and initial and boundary conditions.

Example 1.5 *Water quality control of a river segment*

Water quality in a river segment is affected by the quality of inflow water from its upstream boundary. Assume that the purpose of constructing a model is to manage the water quality along the river segment. If the river is relatively narrow and shallow, only the cross-sectional average concentration along the river segment needs to be known. In this case, we can use the following 1-D advection–dispersion–reaction model (Schnoor 1996):

$$\frac{\partial C}{\partial t} - \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) + v \frac{\partial C}{\partial x} + RC = 0, \quad (1.1.6)$$

with initial and boundary conditions

$$C(x, t) \big|_{t=0} = C_0(x), \quad C(x, t) \big|_{x=0} = C_{in}(t), \quad \frac{\partial C}{\partial x} \big|_{x=L} = 0. \quad (1.1.7)$$

The governing equation (1.1.6) is a second-order parabolic PDE derived from the mass conservation and Fick's law. In this model, the cross-sectional average concentration distribution, $C(x, t)$, is the state variable, and the concentration of inflow water, $C_{in}(t)$, is the control variable. Other parameters and variables include the flow velocity v ; the dispersion coefficient D , which represents not only the molecular diffusion, but also the effect of the small-scale turbulent flow; the linear reaction rate constant R ; the length of the river segment L ; and the initial concentration distribution C_0 .

If the reaction is nonlinear, the reaction term will depend on the concentration. For uniform and steady-state flow, the velocity $v(x, t)$ in (1.1.6) can be measured. When the river flow is nonsteady and nonuniform, however, $v(x, t)$ must be calculated using the river flow model presented in Example 1.4.

Example 1.6 *Modeling groundwater flow in an unconfined aquifer*

Transient flow in an unconfined aquifer is governed by the following second-order parabolic PDE by invoking the Dupuit–Forchheimer approximation, which states

that water-level variation in the horizontal direction is negligible and head distribution in the vertical direction is hydrostatic (Bear 1979):

$$S_y \frac{\partial h}{\partial t} = \nabla \cdot [K(h-b)\nabla h] + Q_R - \sum_{i=1}^{N_w} W_i \delta(\mathbf{x} - \mathbf{x}_i), \quad i = 1, 2, \dots, N_w. \quad (1.1.8)$$

In (1.1.8), $h(x, y, t)$ is the water table elevation; W_i is the pumping rate from the i th well located at \mathbf{x}_i ; N_w is the total number of wells; $\delta(\mathbf{x} - \mathbf{x}_i)$ is the Dirac delta function; Q_R is the net recharge rate per unit area; S_y is the specific yield; K is the hydraulic conductivity; and b is the bottom elevation of the aquifer. To solve the state variable $h(x, y, t)$ from (1.1.8), we must have the following information: control variables W_i and Q_R ; system parameters S_y , K , and b ; the geometry of flow region Ω ; the initial condition $h(x, y, 0) = f_0$ over Ω ; and the boundary conditions $h|_{\Gamma_1} = f_1$ and $-K(h-b)\nabla h \cdot \mathbf{n}|_{\Gamma_2} = f_2$ along the entire boundary of Ω , where f_0 , f_1 , and f_2 are known functions, Γ_1 is the given water-level boundary condition, and Γ_2 is the given flux boundary section with \mathbf{n} being its unit normal vector. In practice, the above-mentioned conditions and parameter values may not be known completely and exactly.

Example 1.7 *Cleanup of a contaminated aquifer*

Pump-and-treat is a remediation technology commonly used in the remediation of contaminated aquifers. To determine pumping locations and rates, we can couple a groundwater flow model, such as the one given in *Example 1.6*, with a 2-D advection–dispersion model (Bear 1979):

$$\frac{\partial \theta C}{\partial t} = \nabla \cdot [\theta \mathbf{D} \nabla C] - \nabla \cdot (\theta \mathbf{V} C) - S(C) \quad (1.1.9)$$

subject to initial and boundary conditions

$$C|_{t=0} = g_0, \quad C|_{\Gamma_1} = g_1, \quad -(\mathbf{D} \nabla C - \mathbf{V} C) \cdot \mathbf{n}|_{\Gamma_2} = g_2. \quad (1.1.10)$$

In this model, the state variable, $C(x, y, t)$, is the contaminant concentration in the aquifer; θ is the effective porosity; $\mathbf{V}(x, y, t)$ is the average linear velocity determined using the hydraulic head $h(x, y, t)$ solved from the flow model; \mathbf{D} is the hydrodynamic dispersion coefficient (a tensor); and $S(C)$ is a sink/source term accounting for chemical reaction, decay, and adsorption processes. In the auxiliary conditions given in (1.1.10), g_0 , g_1 , and g_2 are known functions, and other notations are the same as those given in *Example 1.6*.

Hydrodynamic dispersion accounts for the effects of mechanical dispersion and molecular diffusion in porous media. Mechanical dispersion is caused by the difference between the average velocity in the macroscopic level and the distributed

velocity in the microscopic level. For an isotropic porous medium, the dispersion coefficient \mathbf{D} depends on the flow velocity \mathbf{V} , longitudinal dispersivity α_L , and transverse dispersivity α_T , according to

$$\begin{aligned} D_{11} &= \left(\alpha_L V_1^2 + \alpha_T V_2^2 \right) / |\mathbf{V}| + \tau D_d, \\ D_{12} &= D_{21} = (\alpha_L - \alpha_T) V_1 V_2 / |\mathbf{V}|, \\ D_{22} &= \left(\alpha_T V_1^2 + \alpha_L V_2^2 \right) / |\mathbf{V}| + \tau D_d, \end{aligned} \quad (1.1.11)$$

where D_{11}, D_{12}, D_{21} , and D_{22} are elements of the tensor \mathbf{D} , V_1 and V_2 are components of \mathbf{V} and $|\mathbf{V}|$ is its magnitude, D_d is the molecular diffusion coefficient, and $0 < \tau < 1$ is a coefficient related to tortuosity of flow paths in the porous medium. Detailed derivation of the advection–dispersion equation (1.1.9) can be found in Bear (1979) and Sun (1996).

Major assumptions underlying (1.1.9) include the following: (i) Upscaling of the flow field from the microscopic level to the macroscopic level is valid; (ii) Fick’s law is applicable for hydrodynamic dispersion; (iii) the Dupuit–Forchheimer assumption is valid; and (iv) a 2-D mass transport model is acceptable; if not, a 3-D coupled flow and contaminant transport model should be constructed.

When the control variables (i.e., the extraction locations and rates) are changed in the flow model, the flow field \mathbf{V} and the dispersion tensor \mathbf{D} in the mass transport model are changed accordingly, which cause the change in concentration distribution. The effect of pump-and-treatment can thus be predicted.

Example 1.8 Large-scale emission management

In large-scale air pollution modeling, the concentration distribution of a chemical compound is governed by a mass balance equation that takes account of the effects of advection, dispersion, deposition, emission, and chemical reactions (Zannetti 1990). If N_c chemical components are involved, the model consists of the following N_c -coupled PDEs:

$$\frac{\partial C_i}{\partial t} - \nabla \cdot (\mathbf{K} \nabla C_i) + \nabla \cdot (\mathbf{V} C_i) + k_i C_i - E_i + Q_i(C_1, C_2, \dots, C_{N_c}) = 0, \quad (1.1.12)$$

$$(i = 1, 2, \dots, N_c)$$

where $C_i(\mathbf{x}, t)$ is the concentration distribution of the i th chemical compound, \mathbf{K} is a dispersion tensor that accounts for the effect of small-scale airflow, \mathbf{V} is the average velocity of airflow at the large scale, k_i is the deposition rate of the i th compound, $E_i(\mathbf{x}, t)$ is the emission source strength, and Q_i is the function of chemical reactions between the i th compound and other compounds.

An important assumption used in deriving (1.1.12) is the so-called K -theory that is similar to Fick’s law. It states that the large-scale dispersion flux, caused by the difference between the small-scale airflows and the average airflow at the large scale, is proportional to the concentration gradient, with the dispersion tensor \mathbf{K} being

the proportion coefficient. In the case of steady-state airflow, we can use a diagnostic model, for which the velocity \mathbf{V} in the advection term is simply obtained by interpolation and extrapolation of meteorological measurements. When the purpose of model construction is to predict the development of a contaminant plume under transient airflow condition, a prognostic model is needed where the velocity \mathbf{V} is obtained by solving a dynamic meteorological model.

The air pollution model consists of N_c -coupled, second-order parabolic PDEs and their auxiliary conditions. In this model, the N_c concentration distributions are state variables, the emission source strengths are control variables for managing the air quality, and others are system parameters that can be calculated by empirical formulae or estimated by data. The components of airflow velocity and dispersion tensor may contain significant uncertainty. ■

From the examples presented thus far, we can draw the following conclusions:

- The governing equations of a physics-based model are derived from fundamental physical and chemical laws and, thus, can be used in any case; however, the values of system parameters and auxiliary conditions are case dependent and need to be determined on a case-by-case basis.
- Different governing equations may be derived for the same problem when different assumptions are involved. Making assumptions and simplifications is essential in EWR modeling because we cannot construct a model that characterizes a EWR system exactly in all aspects and at all scales. In fact, the process of choosing appropriate assumptions and determining the appropriate level of model complexity is also case dependent and is oftentimes an art in EWR modeling.

As a solid example of the above conclusions, we see that models of mass transport in rivers (Example 1.5), porous media (Example 1.7), and air (Example 1.8) all share the same mathematical form, namely the advection–dispersion–reaction equation

$$\frac{\partial C}{\partial t} = \nabla \cdot [\mathbf{D} \nabla C] - \nabla \cdot (\mathbf{V} C) - R(C) + E, \quad (1.1.13)$$

which is subject to appropriate auxiliary conditions. However, the dispersion coefficient \mathbf{D} has different physical explanations and magnitudes in different problems and the same for the reaction term $R(C)$ and sink/source term E . Equation (1.1.13) may become nonlinear when \mathbf{D} or \mathbf{V} is dependent on C (in the case of viscous flow) or when $R(C)$ is a nonlinear function.

1.1.3 General Form and Classification

Although different systems and models appear in different EWR fields, all of them can be expressed in the following general form:

$$\mathcal{L}(\mathbf{u}, \mathbf{q}, \mathbf{p}, \mathbf{b}) = \mathbf{0}. \quad (1.1.14)$$

Equation (1.1.14) is called an operator equation (see Appendix A). It may consist of one or a set of algebraic equations, integral equations, ODEs, or PDEs that represent the quantitative relationships between state variables and other variables or parameters of the system under consideration. In (1.1.14), \mathbf{u} , \mathbf{q} , \mathbf{p} , and \mathbf{b} are state variables, control variables, model parameters characterizing the internal properties of the system, and boundary parameters in both spatial and temporal domains, respectively. They can be scalars, vectors, functions, and vector functions.

A classification of mathematical models is provided below:

- *Single-state model* versus *multistate model*, depending on whether the number of state variables is one or more than one.
- *Linear model* versus *nonlinear model*, depending on whether or not all model equations are linear.
- *Deterministic model* versus *probabilistic* (or *stochastic*) *model*, depending on whether random variables appear in model equations.
- *Lumped parameter model* versus *distributed parameter model*, depending on whether or not spatially varying parameters are involved in model equations. When the spatial variability of a system can be ignored or averaged, the system can be regarded as a point and simulated by a lumped parameter model. A distributed parameter model is represented by PDEs, while a lumped parameter model is represented by ODEs.
- *Steady-state model* versus *transient model*, depending on whether or not the time variable is involved in model equations.
- *Physics-based model* versus *data-driven model*, depending on whether or not physically based parameters appear in model equations.

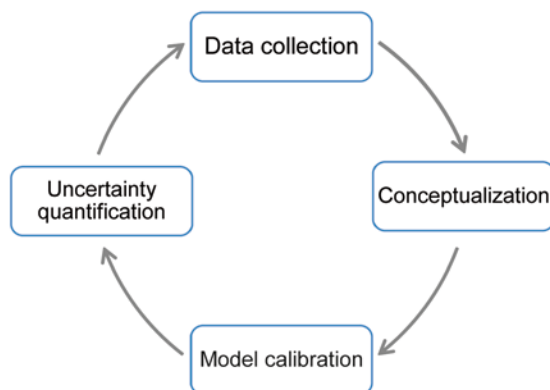
All model types listed in the above exist in EWR modeling, as we have already seen in Sect. 1.1.2. The state of a EWR system may be characterized by more than one correlated state variables, its structure is usually inhomogeneous, the relationships between its variables can be nonlinear, its state variables and parameters may depend on both locations and time, and its internal structure and external conditions are usually uncertain. As a result, (1.1.14) can be a highly complex mathematical model for a EWR system. This book focuses on the construction and calibration of such highly complex models.

1.1.4 Model Construction Process

A typical process of constructing an EWR model consists of the following steps (Fig. 1.1):

- *Data collection*: Collect all existing data that can provide information for model construction and calibration, such as measurements of state variables, control variables, and system parameters, and the knowledge of experts; site-specific field campaigns may be designed and conducted to acquire additional information.

Fig. 1.1 Major steps of model construction



- *Conceptual model development*: Select an appropriate model structure and determine the model equations based on the underlying physical/chemical processes, analysis of the collected data, and the assumptions made for model simplifications.
- *Model calibration*: Adjust the structure of the conceptual model and identify its parameters so that model outputs can fit the collected data.
- *Uncertainty quantification*: Estimate the reliability of the constructed model when it is used for prediction and decision support.

Among the four steps, the data collection step is the basis of model construction. Without sufficient data, no one can construct a useful model. The conceptualization step is probably the most challenging step for a modeler. A model should be an appropriate simplification of a real system. If the model is oversimplified, important characteristics of the system may be lost, while if it is overcomplicated the model cannot be well calibrated because of data insufficiency. Therefore, the development of a conceptual model is regarded as an evolving process through which the conceptual model is adjusted to reflect newly gained knowledge. In the model calibration step, the model structure is corrected and model parameters are modified through fitting the model outputs to observed data. Model calibration is the key to successful modeling, but can be very challenging. A large fitting residual, of course, is unacceptable, but a small fitting residual does not necessarily mean that the model is acceptable. In the latter case, we can only say that the model cannot be rejected, and that is why we need the additional uncertainty analysis step to assess the reliability of the calibrated model before it is used for prediction and decision making. Assessing the reliability of a nonlinear and complicated model is another challenging problem in model construction. When the calibrated model is deemed to be unreliable, new data must be collected, and the above steps must be repeated. As a result, the model construction process forms a *closed loop* (see Fig. 1.1), as opposed to the *open-loop* process in which all steps are done only once. The construction of a useful EWR model can thus be both time-consuming and expensive.

As described in the remaining sections of this chapter, three common problems are solved repeatedly during a model construction process: the forward problem for simulation and prediction, the inverse problem for model calibration and parameter estimation, and the uncertainty quantification problem for reliability assessment.

1.2 Forward Solution

1.2.1 The Forward Problem

In the forward problem, the model equation (1.1.14) is solved to find the unknown system states \mathbf{u} for given \mathbf{q} , \mathbf{p} and \mathbf{b} . The forward solution forms the basis of model study. The general form of a forward solution can be represented by

$$\mathbf{u} = \mathcal{M}(\mathbf{q}, \mathbf{p}, \mathbf{b}), \quad (1.2.1)$$

where \mathcal{M} is a mapping from $(\mathbf{q}, \mathbf{p}, \mathbf{b})$ to state variables \mathbf{u} . Mapping is an extended concept of function when its variables are functions (see Appendix A). Analogous to computer programming, $\mathcal{M}(\cdot)$ can be seen as a subroutine with \mathbf{q} , \mathbf{p} , and \mathbf{b} as its inputs, and \mathbf{u} as its outputs. The forward solution provides an explicit representation of the “excitation–response” relationship for the system being modeled.

In some simple models, such as the models in *Examples 1.1 and 1.3*, the forward solution is given explicitly. For most EWR models, however, state \mathbf{u} appears in the model equation implicitly, and one or more equations must be solved to obtain the forward solution.

1.2.2 Solution Methods

The solution of the forward problem has been extensively studied in mathematics and engineering. Analytical and numerical methods for solving linear and nonlinear algebraic equations, integral equations, ODEs, and PDEs can be found in many mathematical textbooks for scientists and engineers (e.g., Polyanin and Manzhirov 2007; Hoffman 2001; Lapidus and Pinder 1982; Beven 2012; Celia and Gray 1992; Sun 1996; Helmig 1997). In most cases considered in this book, an EWR model is a distributed parameter model expressed by one or more PDEs (i.e., \mathcal{M} is physically based). Typical PDEs appeared in EWR modeling include the elliptic PDEs used to describe steady-state flow processes, the parabolic PDEs used to describe transient flow and transport processes, the second-order hyperbolic PDEs used to describe wave or oscillation processes, and the first-order hyperbolic PDEs used to describe pure advection processes. Analytical and numerical methods for solving PDEs can be found in many books on EWR modeling (Bear 1979; Sun 1996; Zlatev 1995;

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