

# Chapter 1

## Introduction

*Urban water management is the engineering discipline with technical and professional responsibility for the design and operation of the extensive structures, installations, and institutions that are necessary for modern society to deal efficiently and comprehensively with water in urban areas. In the training of engineers, the first concern is to instill an understanding of the principles of the functioning of the entire technical system of urban water management. This is the primary goal of a first lecture series on urban water management (Gujer, 2002). The present text assumes that students have such a basic understanding and will introduce a set of methods that support productive and successful work in this engineering discipline.*

Thus the focus of this text is on scientific methods that are useful in the analysis and prediction of the behavior of the systems, processes, and operations used in urban water management. Specific topics such as physicochemical or biological treatment of water are explicitly not the subject of this text. However, working efficiently with these topics requires the methods introduced herein.

### 1.1 Goal and Content of This Text

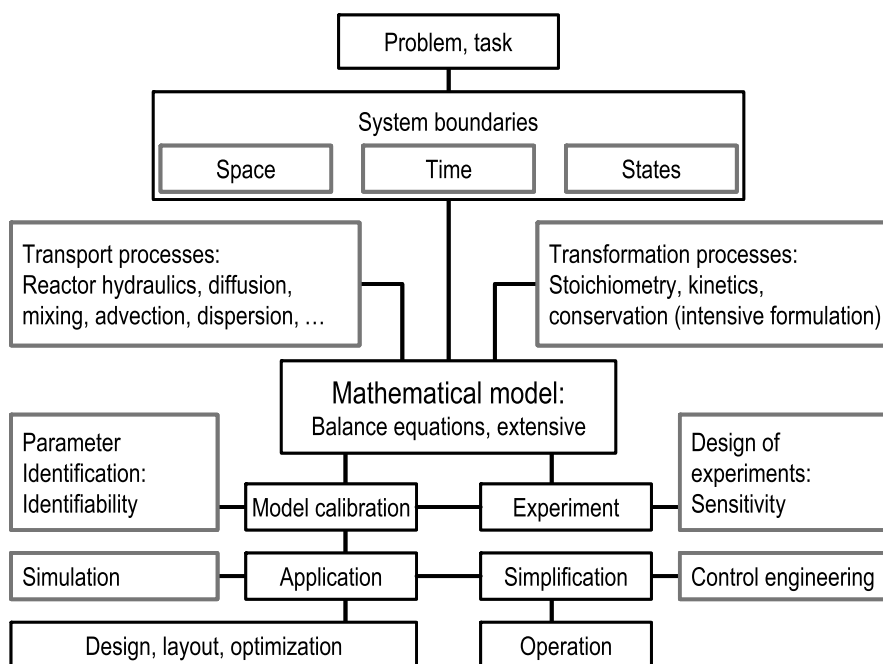
In urban water management we frequently concern ourselves with dynamic, i. e., time-dependent technical and natural systems, which we analyze with the aid of mathematical models. Causes of the dynamics are diurnal and seasonal variations as well as random events such as rain. Typically our problems require that we deal with many different materials and processes and analyze rather complex technical systems.

This text aims to introduce the methodological basis for the development and application of dynamic mathematical models. The goal is to introduce the basics such that the student will be able to develop and apply his or her own models and

plan and interpret associated experiments and data. This will lay the groundwork for the future development of more complicated models and independent acquisition of his or her own preferred methods.

Figure 1.1 shows a simplified flow scheme for the treatment of problems, starting from a question and ending with an answer:

- We start from a task and an associated question that refers to a natural or technical system from the real world.
- First we delimit this system from its environment. This demarcation is an abstraction step which considers that the environment may affect the system under consideration. However, the system may not affect the environment such that there is feedback to the system again. Therefore effects of the system on the environment do not have to be considered. This demarcation refers to space, time, and the spectrum of state variables (state variables are time-dependent values that are important to the problem under consideration).
- In order to model the system mathematically, we need an understanding of the transport processes (here, primarily the topics of material flux, reactor hydraulics, mixing, advection, dispersion, and diffusion will be introduced). Transport processes do not change the materials; they affect only the concentration of the materials that are available at a particular location and time.



**Fig. 1.1** From a question to a model to a solution of the problem. In *gray*: The different tools and themes of this text

- Chemical, biological, and to some extent physical processes convert educts into products. With the help of kinetics we characterize how the local environment affects the rate of these processes. Stoichiometry indicates the ratio in which educts are converted into products. Conservation laws provide us with a priori information, which is used to simplify our task.
- The mathematical model is now compiled in the form of a set of equations (with dynamic systems usually as ordinary and partial differential equations). For this we use material balance equations that combine the effects of the environment, transport, transformation, and changes in the state variables. The model should be simple, but describe the relevant phenomena with sufficient accuracy.
- Now, the parameters of the model must be determined, typically based on experiments or our professional experience. In addition, we will plan experiments which react sensitively to the parameters. For this we use the methods of sensitivity analysis.
- In order to calibrate the model (adapt it to experimental results) and to validate it (gain confidence in its validity), the parameters must be identifiable and identified. For this we make use of experimental observations and possibly nonlinear regression techniques.
- If our question concerns problems in the domain of planning, design, and optimization, the model may now be used with the help of simulation (usually based on the numerical solution of a system of differential equations).
- If the question concerns the operation of a system, the model equations are often simplified, and methods from control engineering will be applied.

The scheme, introduced here in the form of an abstract analysis will be developed systematically in the text and explained with many examples. Sophisticated concepts cannot be evaluated without a detailed understanding of the methods and tools for urban water management that are introduced here.

While the problems that we deal with in urban water management change continuously, the methods that we use are fairly stable. Classical methodical textbooks, in particular from chemical and process engineering, partly go back to the 1950s and 1960s.



## Chapter 2

# Modeling and Simulation

*It is a characteristic of environmental engineering that we must frequently predict the behavior of extensive, complicated systems with highly variable boundary conditions. Often, important data and information are missing. With models that allow us to transfer experience from one system to another, we can partially compensate this lack of information.*

*Thus, modeling is an important aspect of our profession — simulation makes use of these models and permits us to make statements about the expected behavior of rather complicated systems. To simulate means to predict the behavior of a system of interest with the help of typically numeric solutions of model equations. We answer questions such as “What would be, if ...?”*

### 2.1 System, Model, Simulation

We speak of a *system*, if some objects and their interactions are separated by a plausible demarcation from their environment (i. e., from the complex reality). The objects and interactions that are of importance relative to the question posed must be part of the system. All other objects and interactions are to lie outside of the system boundaries. We then describe such a system with the aid of mathematical *models*, which we can analyze instead of the real system. Finally, we will apply to the real system what we learnt from the behavior of the models.

We differentiate between physical models (a model railway, a geographical map, a pilot plant, etc.) and abstract, usually mathematical, models. In this text abstract models are of interest.

*Modeling* always starts with a process of abstraction: we reduce system complexity in view of the question posed. Only important processes, state variables, parameters, and interactions are maintained. We will first develop qualitative, verbal descriptions (models), which can then be transformed into quantitative, mathematical models used to describe system behavior.

Simulation means to experiment with abstract models in order to answer questions like “*what would be, if ...?*”. With the aid of mathematical methods we analyze the possible behavior of a system. We will then use what we learn from model predictions to design, optimize, and operate real-world systems.

## 2.2 Models in Natural and Engineering Sciences

*Research in natural sciences is the attempt to fathom the mechanisms that lead to the observed behavior of a natural system. Engineering has the task to plan, design, realize, and operate systems based on scientific knowledge, and thereby to achieve a set goal with the least possible effort.*

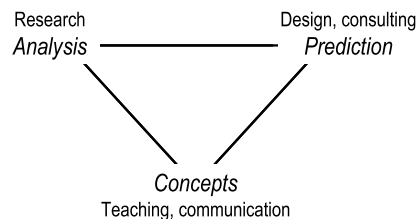
It is common to both disciplines that they are successful only by abstractions or models of reality. The task of the natural scientist is to develop models that provide an ever-improving understanding of reality. The method of the engineering sciences is to compile models which, at small expense, provide valid statements about the problem at hand. Thus, in environmental engineering the focus is not on modeling per se, but rather on developing models that serve a purpose. In the environmental natural sciences, the development of models that uncover interactions may well be the actual goal of the work.

Apart from analysis (research) and prediction (project engineering, consulting), we also use models in teaching of concepts and communication of relationships (Fig. 2.1). Here the models are encapsulated knowledge that we can discuss in an internationally standardized and uniform language (mathematics).

## 2.3 Types of Mathematical Models

In the context of this text, we are interested primarily in the following groups of models:

- *Deterministic models* assume that the behavior of a system is clearly determined by its present condition and the future external factors of influence. Given the same initial and boundary conditions, a deterministic model will always lead to the same result. This is in contrast to *stochastic models*, which consider



**Fig. 2.1** Different tasks and goals of modeling

also uncertainties in the model parameters and possible random fluctuations of external variables and thus, even with defined initial conditions, lead to uncertain future behavior.

- *Dynamic models* make statements about the time-dependent development of a system, i. e., the future conditions of a system can be assigned to the time axis. *Static systems* do not make a statement about temporal development. They may well consider changes of external factors, but they do not allow prediction of the temporal transition from one condition to the next. The concept of *steady state* describes the situation of a static system.
- *Spatially discrete models* make statements about subsystems that are considered to be well mixed, and where gradients of the state variables are not modeled; in dynamic models they lead to ordinary differential equations. *Spatially continuous models* also describe gradients of state variables in space and accordingly lead to partial differential equations. If the transport processes are dominated by one or two directions (the anisotropic case), then we can often limit the models to fewer than three spatial dimensions.
- *Temporally continuous models* lead to differential equations; they regard time as a continuum and make statements about the time course of a system. *Temporally discrete models* lead to difference equations; they make statements only for certain times and do not permit the description of the transition between such times in detail.

**Example 2.1:** The bank account is a temporally discrete system

Interest is credited at regular intervals to a bank account. After the annual credit of the interest, the capital and its increase grow with compound interest: a temporally discrete system. If the bank account were a temporally continuous system, then the interest would be constantly credited (each fraction of a second), thus the interest would rise, because we would receive compounded interest much earlier. The banks naturally noticed this – accordingly, we must typically pay interest for our debt every month, whereas we obtain interest only once a year.

Similarly a small population of organisms that grows in discrete steps, e. g., by cell division and duplication, could be described as a temporally discrete system. However, once the number of organisms is so large that the birth of an individual new organism is no longer noticeable, we usually describe the behavior of the system as temporally continuous.

**Example 2.2:** Models used for dimensioning are usually static models

Historically biological wastewater treatment plants were dimensioned based on a sludge loading rate  $B_{TS}$  (frequently called F/M, the food-to-microorganism ratio). Here, only time-independent values are used and it is not possible to forecast the treatment efficiency on an hourly basis. These design models are static.

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**Example 2.3:** The cascade of stirred tank reactors is a spatially discrete model

If we model a plug-flow type reactor with the aid of a cascade of stirred tank reactors, we select a locally discrete model. We can then only make statements about conditions in the individual reactors of the cascade. The model does not provide intermediate values that might be observed in the real reactor. The resulting model consists of a system of coupled ordinary differential equations. If alternatively we were to use a model with dispersion and advection, then a spatially continuous model would result, and accordingly we would obtain a system of partial differential equations.

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**Example 2.4:** Box models are spatially discrete

In the environmental sciences, we frequently model natural systems with so-called box models, i. e., models that consider a part of the system as a completely mixed, homogeneous box (without internal gradients) and transport processes only at the surface of this box (simple examples of box models are batch reactors or stirred tank reactors).

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**Example 2.5:** Rain events are stochastic events

In the dimensioning of sewers, we use information about the intensity, duration, and frequency (IDF) of rain events, which we compile by using statistical methods. A model rain event is computed with the help of a statistical model and will thus never occur in the form used for the design. However, the characteristics of the rain event that is used have a certain probability of occurring.

The statistical characteristics of the real observed rain event are extracted in the form of a constant, average intensity which afterwards leads in the context of the rational method for design (a deterministic model) to a unique result.

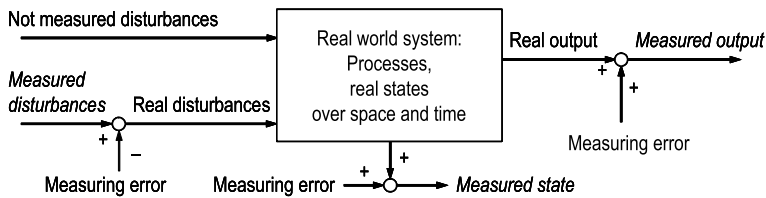
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## 2.4 Systems Analysis

*The tasks of systems analysis are (i) to identify a suitable structure of a mathematical model for the description of the behavior of a system of interest, (ii) to identify the associated parameters of the model, including their uncertainty, (iii) to analyze the mathematical behavior of the models, (iv) to evaluate the quality of the model, (v) to analyze and estimate the uncertainties of the model predictions, and (vi) to plan and design experiments with the best yield of information.*

Figure 2.2 shows an abstract representation of a real-world system. We cannot observe all the external factors that influence the behavior of the system, and those which we can observe are subject to measuring errors. We track the behavior of the real system again with observed conditions and measured output variables,





**Fig. 2.2** Observation of reality and the effect of measuring and observation error

which are also subject to measuring errors. The system itself is subject to processes, which we characterize with abstract mathematical models. The structure of the model that we compile corresponds to our perceptions and concepts. The picture that we create for ourselves for a system is therefore different to a greater or less extent from the unknown reality.

With the aid of systems analysis, we try to grasp the difference between the model prediction and the real-world behavior of the system. Scientific methods are used to keep these differences small and under control. For this we use the following methods:

- The choice of a *model structure* that can cope with system behavior and be identified with the aid of experimental evidence.
- The *estimation of parameters* based on experimental observations given a particular model structure. This is also called system identification. Identified parameters values are burdened with uncertainty.
- *Consideration of sensitivity* will tell us whether the parameters are identifiable and which experiments would yield most information.
- *Error propagation* provides us with estimates of model prediction uncertainties.

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### Example 2.6: Unobservable properties

The distribution of the rain intensity over an urban catchment area can be observed only at great expenditure with the spatial and temporal resolution necessary to describe the discharge behavior of a drainage system reliably. Only a very fine observation grid would yield a reasonably exact picture.

The various organic pollutants in wastewater cannot be described individually, although the detailed composition of the wastewater determines the behavior of the wastewater treatment plant. We must rely on sum or group parameters such as COD and additional experience in similar situations.

On a statistical basis, the water requirement of individuals is well known. We cannot, however, assign an accurate instantaneous value to the requirement of an individual person or a single house.

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## 2.5 Calibration, Validation, and Verification

*No model illustrates the whole of reality. Calibration and validation give us confidence that we can make meaningful use of mathematical models in a limited state and time space. Environmental sciences cannot typically verify their models.*

We *calibrate* a model with a given mathematical structure by achieving an optimum agreement between experimental observations and associated model prediction by adaptation of the model parameters. We *validate* a model by testing its validity in the state and time space required to answer the question posed.

The terms *verification* and *validation* are frequently used as synonyms. However, here we will define verification much more narrowly, using the example of the way in which the law of gravitation has been verified in a very broad sense, such that we can make reliable predictions even for situations where the law has not yet been tested and measurements are not possible. Large and complex models such as those developed and used in the environmental sciences cannot be verified in this sense; we have to neglect too many details that may dominate the behavior of the system in new situations. Typically, we will only validate our models and thereby we are restricted in the possibilities of reliable extrapolation.

*Summary:* We calibrate based on a limited set of experiments. We validate for a limited space of application (a range of temperatures or concentrations, a time period). We verify for a broad field of application without restriction of the validity.

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### Example 2.7: Calibration, validation, and verification

For apples falling from a tree, we can find a simple model that allows us to predict the time  $t$  required to reach the ground as a function of their initial height  $h$ :  $t = k \cdot h^{1/2}$ . Based on many experiments, we can determine the model constant  $k$  (approximately  $0.22 \text{ s m}^{-1/2}$ ). We have calibrated the model. We can easily use this result in order to interpolate, but not yet in order to extrapolate very far. We could definitely not accurately determine the height of an airplane based on dropping an apple, as at high velocities air resistance becomes important.

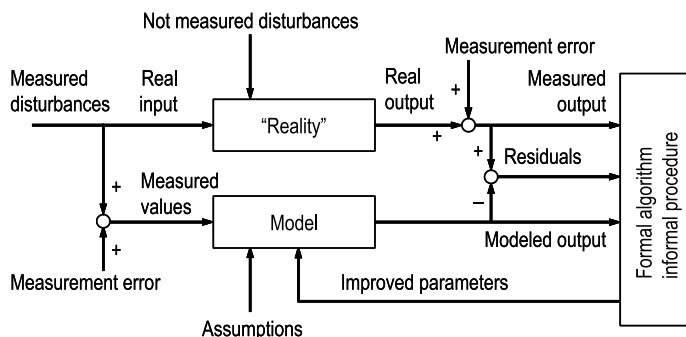
If we now conduct our experiments in a vacuum and find the same value for  $k$  when we instead use a feather or an apple, our confidence increases. The model is now validated for a broad range of application and we would even risk extrapolating somewhat. However, we would certainly not yet board a space ship that is expected to fly us to the moon based on our limited experience.

Only with the gravitation law (and of course a few more details) which can describe many different phenomena and which could be verified from the very small up to the astronomic scale are we willing to risk our life in the space ship. We can then speak of verification and are ready to rely on very broad validity.

In physics the goal is typically to obtain verified models.

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Figure 2.3 introduces a general procedure for the calibration of a mathematical model. We compare measured values from reality, which suffer from measuring



**Fig. 2.3** Calibration of a model. When validating, the improvement of the parameters is omitted

errors, with the predicted values from the model, which are computed based on disturbances (external influences) that likewise suffer from observation errors. With the help of a formal or informal (trial-and-error) procedure, we improve the values of the model parameters until we reach sufficiently good agreement between reality and the prediction of the model.

In validating a model, we frequently use observations of the real system that were not used for the parameter estimation (calibration). If these observations cover the space in which we want to use the model, and the comparison between the prediction and observation is satisfactory, we regard the model as validated for the application. In order to improve the reliability of parameter estimation, it is advisable to include now the data that was used for validation and re-estimate the parameters.

Verification is not an important procedure in environmental engineering sciences.

## 2.6 Model Structure

If we do not succeed in calibrating a model with sufficient security (accuracy), then we must improve the mathematical structure of the model. We may have chosen too simple a mathematical model, we may have neglected important processes, or we may have chosen mathematical expressions that cannot capture the properties of the individual processes. In addition, problems may arise from parameters that are not identifiable based on the experimental evidence at hand.

No scientific procedure guides us in the development of a suitable model structure; rather we have to rely on the application of our professional knowledge, our technical expertise, and the application of scientific findings. Later (Sect. 2.8, and Chap. 12), we will get to know suitable tools and methods that will support us and facilitate this task.

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**Example 2.8:** Air resistance in the law of falling objects

If we want to apply the law that we developed for the description of the falling apple in Example 2.7 to a feather in the wind, we will obviously not succeed. Neglecting the resistance of air is in this case of such importance that we must adapt the model structure in order to obtain a model that can reasonably be calibrated.

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## 2.7 Simulation

*The use of mathematical models to answer questions such as “What would result, if ...?” is called simulation. In a simulation we typically proceed from a validated model.*

Frequently, it is too expensive, illegal, or impossible, to run experiments with the plants or systems that we plan, design, build, and operate because:

- Physical models (pilot plants) are expensive, time consuming, and difficult to operate.
- Experiments can endanger humans (drinking water) or the environment (wastewater), if we leave our field of expertise.
- Natural systems (running waters, lakes, groundwaters) cannot be endangered.
- Rain cannot be imitated in real systems.

With the aid of simulation, we can investigate the behavior of the real world or analyze results from pilot plants based on mathematical models. We can even make a prediction for the circumstances under which a certain danger will arise, etc.

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**Example 2.9:** A definition of the term “simulation”

Many definitions exist. The VDI guideline 3633 provides the following definition (translated from German):

“Simulation is emulation of a system with its dynamic processes in an experimentable model in order to arrive at results which are transferable to reality”.

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**Example 2.10:** Real-time simulation

In large cities the behavior and control of sewer systems are increasingly based on “real-time” simulations of rain events. With the help of weather radar and many signals from the sewer system, the behavior is simulated and the underlying model is calibrated. With a calibrated model it is then possible to simulate different control strategies. The results of such scenarios are then the basis for operators to take decisions for manual interference.

Here calibration with the latest available data is sufficient, because the extrapolation extends only over a short period of time.

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**Example 2.11:** Simulation in hydrology

With hydrological models, prognoses are made for the development of flood conditions in the lowland areas of rivers. This provides early warnings of upcoming dangers.

After an accidental pollutant discharge into a river, simulation programs are used to predict the propagation of the pollutant. This provides early warnings that allow water withdrawals for water supply purposes to be suspended.

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**Example 2.12:** Simulation in process engineering

Today, the performance of entire wastewater treatment plants under variable hydraulic and pollutant loads is simulated in the context of plant design. In addition simulation is used to develop new control concepts for such plants.

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**Example 2.13:** Flight simulators

Pilots are trained in simulators, because it is cheaper than the real thing, and because dangerous situations that in reality would be too risky to consider are available.

Sitting in front of a personal computer (PC) even laypeople can obtain a realistic picture of the task of a pilot from a simulation program.

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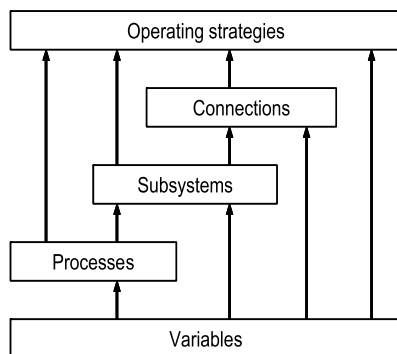
## 2.8 Components of a Model

Today, technical and natural systems in engineering or natural sciences are frequently modeled with systems of algebraic equations as well as ordinary and partial differential equations. These model systems consist of structural components whose characteristics are discussed here. We must strictly differentiate between the real-world system and its mathematical model (a picture). Here we concern ourselves only with the models; however, the individual structural components have of course their parallels in the real world.

### 2.8.1 *Structural Components of a Mathematical Model*

Figure 2.4 shows the structural components of a mathematical model, as they are usually applied in the description of aquatic systems (and many other systems). The arrows suggest the order in which these structural components are defined when a new model is compiled. In detail these elements include:

**Fig. 2.4** The most important structural components of a mathematical model. The arrows suggest the order of the definition of the individual elements (extended from Reichert, 1998)



## Variables

With the variables, we connect numeric values that may be constant or may change with time and/or over space. It is the numeric values of the variables which we must enter and adapt for a specific system, or which we examine, analyze, or display in detail. We distinguish the following types of variables:

- *Intensive properties* are variables that are defined for a specific location and are independent of the size of the system, e. g., concentrations, temperature, flow velocity, and viscosity. *Extensive properties* are proportional to the size or mass of the system and therefore always refer to a certain system, e. g., flow, volume, diameter, length, mass, and energy.
- *System variables*: Statements about the condition of a system always refer to a certain time and a certain location in a specific subsystem. We call the variables that allow us to localize a specific condition in time and space system variables. Typical system variables are time, local coordinates, and the designation of the subsystems. Depending upon the type of the model (stationary, homogeneous, discrete, etc.) we may neglect some of these variables.
- *State variables* are the dependent variables whose prediction as a function of the system variables is the actual goal of modeling. Examples are concentrations, temperature, flow (not influent), flow velocity, and time-dependent volumes.
- *Disturbances* are factors or properties that affect a system from the outside and which we (in the context of our investigation) cannot influence. Examples are influents and their pollutant content or measuring error.
- *Initial and boundary conditions*: In order to be able to solve ordinary and partial differential equations, we must provide absolute values and possibly derivatives for state variables at specific times and locations. These can result from data (possibly as model parameters which must be identified) or may be chosen as the steady (not time-dependent) state of the system under mean operating conditions. A steady state may be obtained with the help of numeric integration (relaxation) of the relevant model equations.

- *Parameters* are variables whose absolute value must be known before model equations can be solved. Examples are fixed volumes, kinetic rate constants (e.g., a growth rate), stoichiometric ratios (e.g., a yield coefficient), hydraulic variables (e.g., wall roughness or viscosity), and material properties (e.g., Henry or diffusion coefficients). It may be necessary to identify kinetic or stoichiometric parameters in the course of model identification, but this requires us to provide strategies to choose the absolute values before we solve model equations. System-dependent parameters (volume, flow, diameter, mass, etc.) can typically be specified a priori based on the problem to be solved.
- *Data* are values from observations or measurements in the real system that is to be simulated. These are measured values for which absolute values (subject to measuring error) as well as system variables (time, location, also subject to error) are available. Frequently it is assumed that time and location but not the data are observed free of error.

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**Example 2.14:** System variables

In a batch reactor (a completely mixed model system with neither influent nor effluent), we track the concentration of pollutants (state variables). Complete mixing leads to the fact that we do not expect concentration gradients over the volume. Therefore the space coordinates are omitted as system variables and only time remains.

Models of rivers frequently neglect the region of transverse mixing of pollutants below a sewage outlet. The assumption is that the river is completely mixed in a cross section, but that gradients of state variables remain in the longitudinal direction. Only the longitudinal coordinate and time remain as system variables, and the remaining model is called one dimensional (1D). If mixing across the river is of interest, we have to choose a two-dimensional (2D) model, and only a three-dimensional (3D) model could provide the full details of the mixing process.

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**Example 2.15:** Intensive and extensive variables

The load of pollutants [ $M_S T^{-1}$ ] entering a wastewater treatment plant is proportional to the size of the city that produces the wastewater, and is thus an extensive variable. We cannot transfer the experiences with this specific load to another city of different size. The specific production of pollutants per inhabitant (60 gBOD<sub>5</sub> per person per day) is an intensive property that can be used for the design of different plants.

The sludge loading rate  $B_{TS} = Q \cdot BOD_5 / (V_{AT} \cdot X_{TSS})$  is an intensive property. By dividing the flow  $Q$  by the volume  $V_{AT}$  of the aeration tank it becomes independent of the size of the plant. Experience with a certain sludge loading rate is to a large extent independent of the system and can therefore be transferred to another treatment plant.

The consumption of drinking water in a city (an extensive property) is a characteristic of this city. The water consumption per inhabitant of this city (an intensive property) may, however, be a point of reference for planning in another city.

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## Processes, Sources, and Sinks

Processes result in the physical, chemical, or biological transformation of the properties and location of materials of interest. They determine and change the state of the system. In our models they affect the state variables. We distinguish between transformation and transport processes.

*Transformation processes* produce or consume materials and energy. They characterize sources and sinks that we do not seize with transport processes. We characterize transformation processes as intensive properties, only dependent on time, local state variables, and parameters.

- *Dynamic processes* are material and energy transformation processes that we characterize by stoichiometry and kinetics. The rate of transformation is comparable with the time constants of interest in the analysis of the system.
- *Equilibrium processes* are transformation processes for which the rates of forward and backward reaction are very large in comparison with the time constants of interest in the analysis of the system. Equilibrium is reached when the production and consumption in these processes is very much larger than the sum of all other processes (transport and transformation) that affect these materials. If equilibrium is reached, we do not have to pursue the time dependence of these transformations. Given that time is the only system variable, the state variables involved may be predicted from coupled algebraic equations.

### Example 2.16: Equilibrium process

Many acid–base reactions are very fast. We typically characterize them as an acid–base equilibrium. We could also capture this behavior as a combination of a fast forward and backward reaction.

For the equilibrium:  $\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}^+$  the equation

$K_S = \frac{[\text{HCO}_3^-] \cdot [\text{H}^+]}{[\text{CO}_2]}$  provides us with a relationship between the concentration of

the acid  $[\text{CO}_2]$  and the base  $[\text{HCO}_3^-]$ . In place of this relationship we could also introduce two fast reactions:

Forward reaction:  $\text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{HCO}_3^- + \text{H}^+$  with  $r_{\text{forward}} = k_f \cdot [\text{CO}_2]$ .

Backward reaction:  $\text{CO}_2 + \text{H}_2\text{O} \leftarrow \text{HCO}_3^- + \text{H}^+$  with  $r_{\text{backward}} = k_b \cdot [\text{HCO}_3^-] \cdot [\text{H}^+]$ .

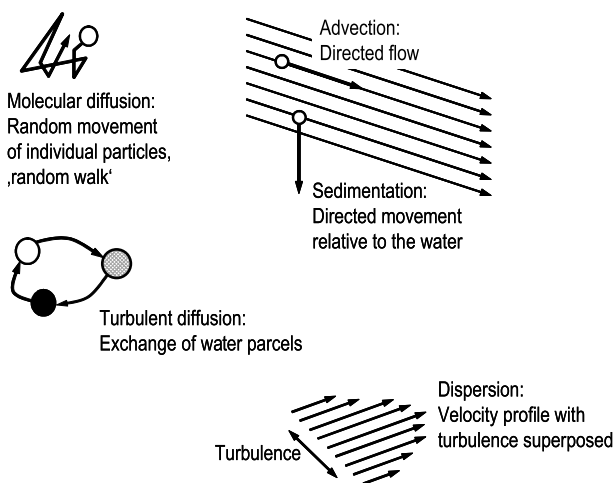
In equilibrium the two reaction rates are equal ( $r_{\text{forward}} = r_{\text{backward}}$ ). This results in:  $K_S = \frac{k_f}{k_b}$ . If we want to use the two reaction equations in place of the equilibrium,

we can, e. g., select  $k_f$  very large and afterwards derive the required value of  $k_b$  from this relationship. The Berkeley Madonna software provides a special module to enter equilibrium reactions in the form of fast forward and backward reactions.



*Transport processes* bring materials and energy from one location to another, neither changing their quantity or mass nor their kind. Transport processes are directional and are quantified as vector variables. We distinguish between (Fig. 2.5):

- *Advection*, which is a directional transport that affects all materials as well as the surrounding water in an equal way. On the average there is no relative velocity of the materials transported and the surrounding water. We characterize advection by a flow velocity.
- *Sedimentation and flotation*, which characterize the falling or rising of particles due to gravity, buoyancy or a *centrifugal* or *magnetic* force. Unlike advection, the particles move relative to the surrounding water.
- *Dispersion*: If we model a three-dimensional flow field with only one- or two-dimensional models, we must neglect some induced flows and velocity gradients. We can compensate this simplification by the introduction of an additional, locally averaged transport process called *dispersion*: we introduce an additional surrogate transport process that averages transport at a particular time over a certain area (e. g., a cross-sectional area).
- *Turbulence*: As a consequence of the dissipation of mechanical energy eddies arise in the water which we hardly can grasp in all detail. Parcels of water together with their content of materials are exchanged, which results in a transport process. We quantify turbulence for a specific location, averaged over time.
- *Diffusion*: The transport of material resulting from the random movement of individual molecules and small particles (thermal motion) is called diffusion. Diffusion is a characteristic of the transported material or particle size and the surrounding water. We quantify the transport of a material, at a specific location, averaged over time. Diffusion makes a statement about the probability that, within one time period, a particle moves in a certain direction.



**Fig. 2.5** Characterization of the transport processes

*Technical processes and controlled elements or members* are procedures that we control purposefully, based on predefined mainly mathematical rules. Examples are aeration equipment, dosing of chemicals, operation of heat exchangers, flow control, and valve positions.

## Subsystems

Subsystems are defined parts of a system for which we can compile independent models. Frequently models for subsystems are based on *idealized, typed elements*, for which we can describe the transport processes and the boundary conditions mathematically exactly. Therefore we can write the balance equations for the state variables of these subsystems. The model of the entire system can then be developed based on the subsystems. Subsystems can affect the states of the system such that feedback to the subsystems may exist. As a consequence we cannot analyze the subsystem autonomously, but only as a part of the entire system.

- *Ideal reactors*: When modeling technical systems, we use ideal reactors as templates for the models of subsystems. Ideal reactors are defined such that we have an exact mathematical description of their behavior. They are discussed in detail in Chap. 6.
- For the description of natural systems we can use predefined subsystems or compile them, depending upon the problem to be solved. Environmental scientists have a suite of models and programs available which offer such predefined model structures for lakes, 1D, 2D or 3D models for rivers and groundwater, soil columns, activated sludge plants, wastewater treatment processes, etc. Often these models provide predefined transport and mixing processes, whereas the transformation processes must be defined by the user.

## Connections

*Connections (links)* of subsystems are extensive resources; they *transport* materials, energy, etc. (quantified by state variables) from one subsystem to another. Usually we neglect the volume of these connecting elements; accordingly no transformation processes must be considered in these elements. Influent and effluent are links to the environment for which one end is not considered when we analyze a system.

- *Simple connections* lead mass and energy unchanged from one subsystem to the next. In the case of a material flow they are defined, e. g., by the flow rate and the material concentrations contained in it.
- *Recirculations* lead mass flows against the general direction of flow from a later to an earlier subsystem. They typically lead to rather intensive coupling of the mass balance equations of different subsystems.
- *Unions* combine and mix the mass flows from several subsystems and feed them united into a new subsystem.

- *Bifurcations* divide the mass flows in a connection and feed them into several subsystems. It is possible that a bifurcation distributes the different materials contained in the flow in different fractions to the effluents of the bifurcation. An example of a bifurcation is a simple model of a sedimentation tank: the influent is split into sediment (with elevated concentration of solids) and treated effluent (with a reduced concentration of solids).
- *Diffusive connections* describe the mass transport over boundary layers, e. g., as a consequence of turbulence, molecular diffusion, or solubility at surfaces. They contain a forward and an appropriate backward reaction and are typically characterized by *mass transfer coefficients*.
- *Disturbances* are inputs into a system. They cannot be controlled at short notice and are not affected by the system itself.

## Operating Strategies

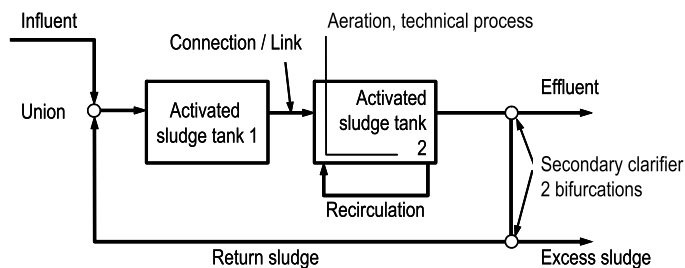
In technical systems we use the existing *degrees of freedom* based on operating strategies in order to reach a desired performance.

- The decisions that operators of technical systems make, are subject to *default operating procedures*; e. g., in the operation of an activated sludge plant we will require a minimum sludge age (solids retention time) to be maintained; in the operation of a sewer system we will require that a certain amount of combined wastewater is directed towards the wastewater treatment plant; or in water treatment we will demand that a minimum concentration of disinfection chemical is maintained over a specified time, etc.
- With the help of *control strategies* and *control engineering*, we can automate the application of *operating procedures*. This requires us to build additional mathematical relations into the systems that make use of control possibilities but decrease the number of remaining degrees of freedom in the operation.

### 2.8.2 Case Study

On the basis of a simple case study, the various structural components of a model (a system) are introduced. Fig. 2.6 shows a schematic for a simple activated sludge system, as could be used to develop a mathematical model. This figure does not want to depict reality but rather the abstraction captured in the model.

The model system is divided into two subsystems (activated sludge tanks), in which the biological transformation processes are active. In these subsystems we must grasp the internal mixing processes. The secondary clarifier, which in reality is a rather large structure, is modeled with zero volume and based on two bifurcations: in the upper layer the clear water that contains soluble materials is separated from the solids, which settle out; in the lower layer the concentrated activated sludge is split into return sludge and excess sludge.



**Fig. 2.6** Flow scheme of a simple activated sludge system that could be the basis for model development. See the text for explanations

Sedimentation and thickening in the secondary clarifier are thus not modeled as transport processes, but captured with a bifurcation, thereby neglecting the time necessary for sedimentation and thickening of the sludge as well as the rather large volume of the clarifier. A total of four links to the environment are included: influent, discharge, excess sludge, and air flow. The material flows in these links do not change the environment in a way that must be considered in the analysis of our system. There is a simple connection between the two subsystems (an aperture), and a technical process (aeration) supplies the required oxygen to the second activated sludge tank. The recirculation inside the second activated sludge tank only has an influence if this subsystem is not modeled as a stirred tank reactor, and thus gradients of state variables in this tank are captured by the model. The return sludge is combined with the inlet and afterwards led into the first reactor.

In this system a set of state variables must be captured to make a comprehensive statement about its performance: oxygen, organic materials, microorganisms, nutrients, temperature, etc. In addition, models for transformation processes (e. g., growth of microorganisms) and associated model parameters such as growth rates (kinetics) and yield coefficients (stoichiometry) are necessary. Moreover, we must define initial and boundary conditions for all the state variables from which our computations proceed. Disturbances (or forcing functions) that affect the system from the outside, such as the influent and its content of pollutants, must be given (we cannot influence these functions at short notice). From the real plant we may have data at our disposal that allow us to calibrate the compiled model. Our goal is to describe the course of pollutant concentrations (state variables) in different locations over time (system variables). This is possible only if we also include the operating strategies, which might be to maintain a constant activated sludge concentration, a steady oxygen concentration, and a fixed return sludge flow rate (degrees of freedom).

## 2.9 Dimensions and Units

*The development, calibration, and validation of models require observations and measurements of state variables. Measurement compares the dimension of variables with a set of fixed standards for mass, time, length, etc. such as the kilogram, second, and meter, respectively, and expresses the result in units.*

Herein variables are defined with their dimension given in straight brackets: [M] for mass (including moles), [L] for length, and [T] for time. Specific values of variables are given in units of grams (g), kilograms (kg), and sometimes moles (mol), meters (m), centimeters (cm), seconds (s), hours (h), and days (d). In a few instances the temperature will have to be expressed either in degrees Celsius (°C) or Kelvin (K).

In systems analysis and mathematical modeling it is good practice *always* to check the homogeneity of the dimensions after a model equation has been derived and the homogeneity of the units once a model is applied (see Example 2.18).

### Example 2.17: Dimension and units of a concentration and a diffusion coefficient

The concentration  $C_{\text{NH}}$  of ammonium in water may be defined as the mass of nitrogen in the form of ammonium per unit volume. Herein it will be introduced as:

$C_{\text{NH}}$  = concentration of ammonium nitrogen [ $M_N L^{-3}$ ]

A specific measured value is given with units such as  $C_{\text{NH}} = 2.4 \text{ gN m}^{-3}$ .

The diffusion coefficient of oxygen in water is introduced as:

$D_{\text{O}_2}$  = molecular diffusion coefficient of oxygen in water [ $L^2 T^{-1}$ ]

Table 4.1 provides specific values for this parameter in pure water at 25°C in two different units:

$D_{\text{O}_2} = 2.42 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$  and  $D_{\text{O}_2} = 2.04 \cdot 10^{-4} \text{ m}^2 \text{ d}^{-1}$ .

Both values express (nearly) the same absolute value of  $D_{\text{O}_2}$ .

### Example 2.18: Homogeneity of dimensions and units in a mass balance equation

Equation (9.8) describes the concentration profile of a pollutant across a spherical activated sludge flock in the format of a differential equation derived from a mass balance:

$$\frac{d^2 C_A}{dr^2} = -\frac{2}{r} \cdot \frac{dC_A}{dr} - \frac{R_A}{D_A}.$$

The definitions of the symbols are as follows:

$C_A$  = concentration of the material A [ $M_A L^{-3}$ ] measured in the units of  $\text{gA m}^{-3}$

$r$  = radius coordinate [L] measured in units of m

$R_A$  = transformation rate of material A [ $M_A L^{-3} T^{-1}$ ] measured in units of  $g A m^{-3} d^{-1}$

$D_A$  = molecular diffusion coefficient of compound A [ $L^2 T^{-1}$ ] measured in units of  $cm^2 s^{-1}$

An analysis of the dimensions results in:

$$\left[ \frac{d^2 C_A}{dr^2} \right] = \frac{M_A}{L^3} \cdot \frac{1}{L^2} = \frac{M_A}{L^5}$$

$$\left[ \frac{2}{r} \frac{dC_A}{dr} \right] = \frac{1}{L} \cdot \frac{M_A}{L^3} \cdot \frac{1}{L} = \frac{M_A}{L^5}$$

$$\left[ \frac{R_A}{D_A} \right] = \frac{M_A}{L^3 \cdot T} \cdot \frac{T}{L^2} = \frac{M_A}{L^5}$$

Obviously the dimensions of the three terms of Eq. (9.8) are equal.

An analysis of the units results in:

$$\left[ \frac{d^2 C_A}{dr^2} \right] = \frac{g_A}{m^3} \cdot \frac{1}{m^2} = \frac{g_A}{m^5}$$

$$\left[ \frac{2}{r} \frac{dC_A}{dr} \right] = \frac{1}{m} \cdot \frac{g_A}{m^3} \cdot \frac{1}{m} = \frac{g_A}{m^5}$$

$$\left[ \frac{R_A}{D_A} \right] = \frac{g_A}{m^3 \cdot d} \cdot \frac{s}{cm^2} = \frac{g_A \cdot s}{m^3 \cdot cm^2 \cdot d}$$

The three terms of Eq. (9.8) are not homogeneous relative to their units. The units of the molecular diffusion coefficient must be changed by multiplying its value by the (dimensionless) factor

$$86,400 s d^{-1} / 10,000 cm^2 m^{-2}.$$

The check of units identifies possible problems in the prediction of absolute values. The check of dimensions identifies possible problems in the derivation of the model equation. However, neither homogeneous dimensions nor units are a guarantee of correct model derivation.

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