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Wastewater Treatment Process Modeling

SECOND EDITION

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Chapter 5

Dedicated Experiments and Tools

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1.0 INTRODUCTION

This chapter provides an introduction to dedicated experiments and modeling tools that may be used during certain phases of the modeling process, particularly the calibration step. The chapter discusses methods for wastewater and biokinetic characterization, approaches for analyzing the mixing behavior of unit processes in water resource recovery facilities (WRRFs), aeration testing, sludge settling characterization, and, finally, a range of tools that support the model calibration itself (i.e., parameter estimation methods to optimize for a range of criteria expressing the quality of a model with respect to acquired data, sensitivity analysis to select the parameters to be estimated, and uncertainty analysis to get a feeling for uncertainty in modeling results). The purpose of this chapter is to give enough background for modelers to decide which method to use and to provide background for the selection of protocols made in the procedures presented in Chapter 8. A wide range of references to literature, guidelines, and method descriptions are provided in this chapter for the reader to refer to for more details.

2.0 WASTEWATER CHARACTERIZATION METHODS

Influent chemical oxygen demand (COD), nitrogen (N), and phosphorus (P) fractions have to be determined according to the model used. This section focuses on measurement of specific characteristics.

Required model inputs (state variables) are typically calculated as fixed percentages (fractions) based on averages of the measured components. However, this is an assumption, and model inputs often vary over the course of a day or week or with weather conditions. Special care should be taken when intermittent industrial loads

are discharged or with seasonal load variations because these atypical conditions may require specific investigations to properly characterize the influent loads.

Table 5.1 provides a list of methods that can be used to characterize wastewater streams in terms of COD fractions. Experience has shown that the proposed methods may lead to different fractions altogether (Fall et al., 2011; Gillot and Choubert, 2010). This also explains why the values obtained through measurements are often modified in the subsequent calibration step.

TABLE 5.1 Experimental methods for COD fractionation of STOWA.[a]

	STOWA	WERF
$COD_{TOT,B}$	Long-term BOD tests	-
S_U	Effluent filtration (0.45 µm)	
	$S_U = 0.9\ COD_{EFF,f0.45}$ (low loaded system) $S_U = 0.9\ COD_{EFF,f0.45}$-1.5 $BOD_{5,EFF}$ (high loaded system)	$S_U = COD_{EFF,f0.45}$
X_U	Deduced from previously determined fractions: $X_U = COD_{TOT} - COD_{TOT,B} - S_U$	SBR operation or full-scale data + calibration of an activated sludge model
S_B	Filtration (0.1µm) $S_B = COD_{f0.1} - S_U$	Flocculation + filtration (0.45µm) $S_B = COD_{ff0.45} - S_U$ OUR-based respirometric methods
XC_B	Deduced from $COD_{tot,B}$ and S_B $XC_B = COD_{TOT,B} - S_B$	Deduced from previously determined fractions: $XC_B = COD_{TOT} - X_U - S_U - S_B$
X_{OHO}, X_{ANO}	Neglected	OUR-based respirometry if required

[a]$COD_{TOT,B}$, total biodegradable COD; S_U, unbiodegradable soluble COD; X_U, unbiodegradable particulate COD; S_B, readily biodegradable (soluble) COD; XC_B, slowly biodegradable (particulate and colloidal) COD; X_{OHO}, ordinary heterotrophic organisms; X_{ANO}, autotrophic nitrifying organisms; $COD_{EFF,f0.45}$, COD of a filtered (0.45-µm) effluent sample; $COD_{f0.1}$, COD of a filtered (0.1-µm) sample; $COD_{ff0.45}$, COD of a sample that is flocculated first and then filtered (0.45 µm); COD_{TOT}, total COD; $BOD_{EFF,f0.45}$, BOD of a filtered (0.45-µm) effluent sample; and $BOD_{5,EFF}$, 5-day BOD of an effluent sample.

(Roeleveld and van Loosdrecht, 2002) and WERF (Melcer et al., 2003) (nomenclature according to Corominas et al. [2010]).

No generally accepted method has been established yet and, therefore, the following steps are recommended (nomenclature according to Corominas et al. [2010]):

- The readily biodegradable fraction (S_B) should be obtained either by respirometry or by physico-chemical methods that include a flocculation step to ensure that the colloidal matter becomes part of the slowly biodegradable fraction.
- The un-biodegradable fraction (S_U) is obtained by COD analysis of a filtered (0.45-μm) effluent sample ($COD_{EFF,f0.45}$).
- The total biodegradable COD fraction of an influent ($S_B + XC_B$) is critical to properly simulate the oxygen demand of the process and its total removal efficiency. To obtain good values of the total biodegradable COD fraction ($COD_{TOT,B}$), long-term biochemical oxygen demand (BOD) measurements or other types of respirometry can be used.

The choice between either a physico-chemical or respirometry method is often based on available equipment and experience. In general, one can say that the former method is easier to carry out (see Chapter 8, Section 2.3.1, for a description and further references). However, it does not measure the biologically relevant property of the wastewater that is used in activated sludge models. Rather, it fractionates COD on the basis of size and not on the basis of rate of biodegradation, which may be important (e.g., for denitrification).

Nitrogen and phosphorus species such as ammonium-ammonia (NH_x-N), nitrite-nitrate (NO_x-N), phosphate (PO_4-P), total phosphorus, total nitrogen, total Kjeldahl nitrogen (TKN), and total soluble fractions are typically obtained through standard analysis. Organic nitrogen and phosphorus fractions are calculated by difference. More information on this topic can be obtained in an early extensive review on characterization methods by Petersen et al. (2003), an International Water Association (IWA) scientific and technical report by Rieger et al. (2012), and a recent critical review of wastewater characterization methods by Choubert et al. (2012).

An important variable in practice is the concentration of total suspended solids (X_{TSS} in model notation). It consists of a volatile part (volatile suspended solids, or VSS) and an inorganic part (inorganic suspended solids; ISS = TSS – VSS). However, the approach for which X_{TSS} is introduced as a state variable in an activated sludge model is not completely described in model publications and needs to be carefully set up. Only then can it become a useful variable that can be linked to TSS measurements.

Respirometry is defined as the measurement and interpretation of the oxygen-uptake rate, r_O, of activated sludge (Spanjers et al., 1998). In general, r_O consists of

the following two components: the exogenous oxygen-uptake rate ($r_{O,ex}$), which is the immediate oxygen uptake needed to degrade a substrate, and the endogenous oxygen-uptake rate ($r_{O,end}$). Different definitions of $r_{O,end}$ appear in the literature. The definition applied here is that the $r_{O,end}$ is the oxygen-uptake rate in absence of readily biodegradable substrate. The exogenous oxygen-uptake rate is calculated from the total uptake rate by subtracting $r_{O,end}$.

Figure 5.1 illustrates the conceptual idea of respirometry. The degradation of substrate S_1 and S_2 (Figure 5.1a) results in a total exogenous uptake rate $r_{O,ex}$

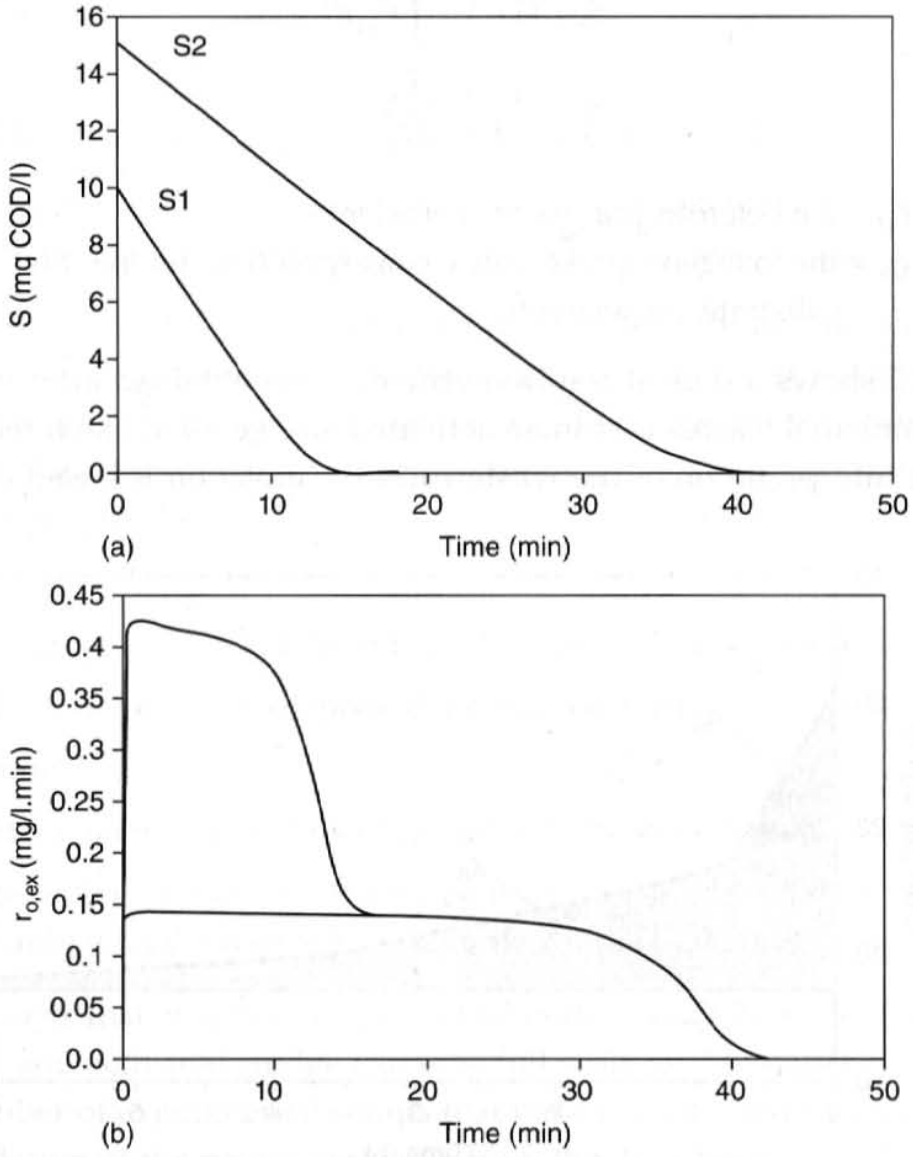

FIGURE 5.1 Degradation of two substrates S_1 and S_2 (a) leading to the conceptual $r_{O,ex}$ respirometric data set and (b) endogenous respiration rates are already subtracted from the total respiration rates measured. (Petersen et al., 2003).

(Figure 5.1b). Figure 5.1b illustrates a typical respirogram (i.e., a time course of respiration rates) with an initial peak in $r_{O,ex}$ caused by oxidation of the most readily biodegradable matter (S_1) followed by, in this instance, one "shoulder" in the $r_{O,ex}$ profile, where component S_2 continues to be degraded. Thus, in this example, the contribution of S_1 and S_2 to total $r_{O,ex}$ can easily be distinguished. It is important to realize that the oxygen demand required to oxidize the substrates can be calculated from the integral under the curve of respiration rates. Biodegradable COD is then calculated as $(1 - Y_H)$ times this integral, that is

$$S_1 = (1 - Y_H) \int r^1_{o,ex} dt \tag{5.1}$$

$$S_2 = (1 - Y_H) \int r^2_{o,ex} dt \tag{5.2}$$

where

Y_H = the heterotrophic yield coefficient

$r^1_{O,ex}$ and $r^2_{O,ex}$ = the oxygen-uptake rates corresponding to the first and second substrate, respectively

Figure 5.2 shows a typical respirometric data set obtained after injection of a sample of municipal wastewater in an activated sludge filled batch reactor. In this instance, the interpretation of the wastewater composition is based on Activated

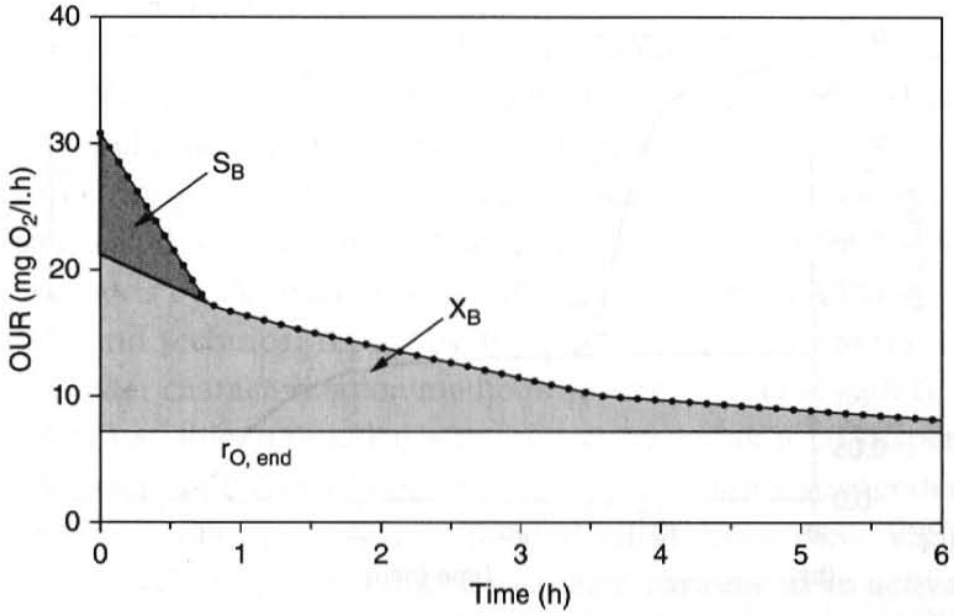

FIGURE 5.2 Typical batch respirometric data set after injection of a municipal wastewater sample in activated sludge. (Kappeler and Gujer [1992]).

Sludge Model No. 1 (ASM1) with S_B (readily biodegradable) and XC_B (slowly biodegradable) fractions differentiated on the basis of their kinetic profiles, XC_B being degraded more slowly. It is important to note that XC_B recorded in such relatively short respirometric experiments does not represent all XC_B, rather, only the faster, degradable part. Longer respirometric experiments are required such as the BOD method proposed by Roeleveld and van Loosdrecht (2002). This method provides the total biodegradable COD that allows calculating XC_B by subtracting S_B (Melcer et al., 2003). Melcer et al. (2003) also describe an alternative method using COD analyses and filtration.

3.0 BIOKINETIC CHARACTERIZATION

The following sources of information can be used to obtain values for the kinetic and stoichiometric parameters of activated sludge models (Petersen et al., 2002):

- Default parameter values from literature. It is important to note that default parameter values are often not the originally published values (called *original parameter values*), but were derived from a consensus-building process in which the profession has agreed that these values are a good starting point for a modeling study.
- Full-scale facility data.
  - Average or dynamic data from grab or time/flow proportional samples
  - Conventional mass balances of the full-scale data
  - Online data
  - Measurements in reactors to characterize process dynamics

Parameter values are obtained through fitting the model until simulation results agree sufficiently with the data (i.e., a calibrated value is obtained).

- Bioassays, that is, different kinds of laboratory-scale experiments with wastewater and activated sludge from the full-scale facility under study. There are a number of experimental setups that have been created that allow the direct calculation of the parameter value from the data. Such value is called a *measured parameter value*. In a number of other methods, a (simplified) model is fitted to the data and one or more parameter values are estimated. In those instances, calibrated values are obtained.

Default kinetic parameters included in activated sludge models generally can describe the performance of most systems treating typical domestic wastewater. However, in some instances, wastewater characteristics and the resulting bacterial community in the biological treatment process are so unusual compared to typical domestic wastewater that the system performance cannot be explained using typical kinetic parameters. Examples of such an instance include a WRRF receiving significant contributions of industrial wastewater or the use of external carbon sources with unusual degradation kinetics (e.g., methanol and glycerol). In these instances, it is beneficial to conduct kinetic studies to better understand the reason for deviations from model predictions and to adjust the relevant model parameters. Kinetic studies can reveal possible causes for unusually slow (or fast) nitrification or denitrification rates.

As mentioned previously, there are two approaches for determining biokinetic parameters (Vanrolleghem et al., 1999). Direct methods focus on specific parameters that can directly be evaluated from the measured data (e.g., nitrification rate deduced from the nitrate data). The values obtained are known as *measured parameter values*. The second approach uses manual or automated optimization methods that use a more or less simplified model that is fitted to the measured data (i.e., calibration). The latter methods use numerical techniques to find parameter values that lead to the smallest deviation between model predictions and measurements. The values obtained are known as *calibrated parameter values*.

Care should be taken when transferring model parameters obtained from laboratory-scale experiments with activated sludge to the full-scale installation (Gernaey et al., 2004). A batch experiment with activated sludge provides much more detailed information about the reaction kinetics compared to full-scale WRRF data, but it may be that the information is reflecting a different behavior than what occurs in the full-scale data. This behavior may be altered because of differences in feeding pattern, environmental conditions such as pH, temperature, mixing intensity or surface-to-volume ratio, or sludge history. Petersen et al. (2003) provide an extensive discussion on this transferability issue.

Two kinetic characteristics that have been the subject of comprehensive method development relate to the nitrification and denitrification rate, as outlined in the following sections. Many dedicated methods have been developed for biokinetic characterization; however, these go beyond the scope of this chapter. The reader is referred to reviews by Melcer et al. (2003) and Petersen et al. (2003) for more information.

3.1 Nitrification Rate

The nitrification rate has often been highlighted as one of the most important factors influencing the required tank volume/aeration time of a WRRF. Even though parameters for nitrification are well documented in the literature, the nitrification rate may be affected by inhibiting or even toxic influent components. Melcer et al. (2003) mentioned two main approaches to determine the maximum nitrifier growth rate using, as mentioned previously, bioassays (a direct method) and full-scale data (interpreted with the optimization method).

3.1.1 Bioassay Methods

Melcer et al. (2003) describes several bioassay methods. The reader is referred to this Water Environment Research Federation (WERF) report for further details on procedures and data interpretation. The following are summaries of the tests:

- Low food-to-microorganism ratio (F/M) tests—nitrifying mixed liquor is combined with influent wastewater containing ammonia. Because of the low F/M, the nitrate production response over time is linear. The main disadvantage of this method is that the nitrifier concentration must be estimated or a sequencing batch reactor (SBR) must be operated for approximately three sludge ages.
- High F/M batch tests—in this test, a relatively small concentration of nitrifying biomass is spiked with ammonia, and the nitrate and nitrite production response is monitored for a period of approximately 4 days (Figure 5.3). Determination of the nitrifiers' maximum growth rate using this test does not require knowledge of the nitrifier concentration, and it does not require the operation of an SBR for an extended period of time.
- Washout test—this test consists of operating a flow-through reactor with nitrifying biomass at a solids retention time (SRT) shorter than the required retention time for nitrification. As with the high F/M tests, the determination of the nitrifier maximum growth rate using the washout test does not require knowledge of the nitrifier concentration or operation of an SBR for an extended period of time.

3.1.2 Simulation of Full-Scale Dynamic Behavior

Determination of the maximum nitrifier growth rate through model simulation of dynamic response behavior can be accomplished by fitting a model prediction to an observed dynamic response in ammonia and/or nitrate and nitrite concentrations

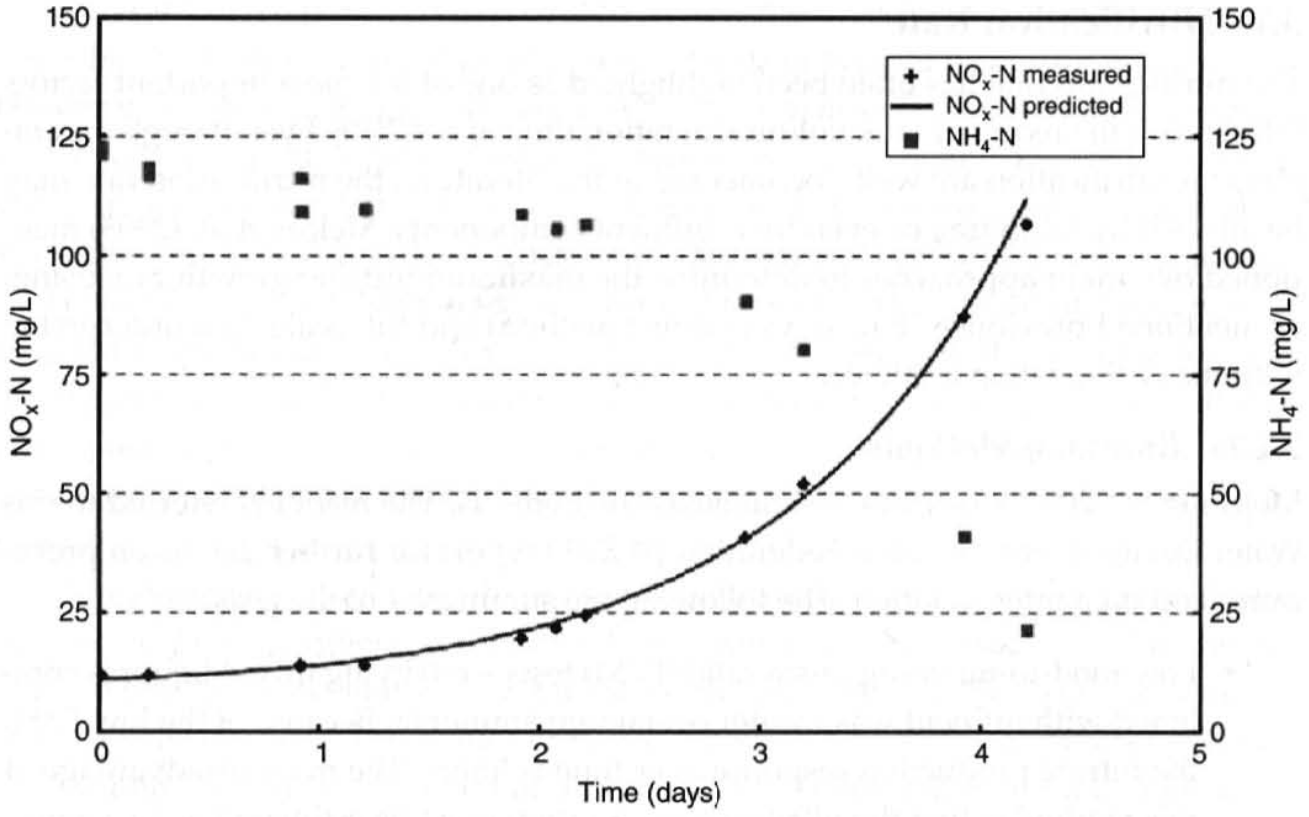

FIGURE 5.3 High F/M batch test results for direct assessment of the nitrifier growth rate. (Melcer et al., 2003).

(Kristensen et al., 1992, 1998). To ensure that the maximum nitrifier growth rate is observed, one must use only those data collected in the absence of limitation because of ammonia, dissolved oxygen, or other substrates. More sophisticated parameter estimation methods (Kristensen et al., 1998; Van Hulle et al., 2007) that simultaneously estimate half-saturation constants for oxygen and ammonia can be applied to deal with these situations.

To maximize the reliability with which parameters can be estimated from experimental data, the principles of experimental design could be applied (Dochain and Vanrolleghem, 2001). While an experiment can be designed using a rigorous model-based procedure, in practical terms it often boils down to selecting those experimental conditions in which extensive dynamics are visible in the variables. The more variation can be seen in the data (either induced by manipulating the process or by external disturbances) the better the estimation will be of nitrification parameters. An example of such simulation-based estimation of nitrification (and denitrification) parameters is given for an SBR study by Corominas et al. (2011).

3.2 Denitrification Rate

Kinetic studies also are common when evaluating specific process changes to achieve or improve denitrification, particularly when alternative carbon sources are to be used. Indeed, unusual carbon sources may result in specific kinetics parameter values that were not considered when the default kinetic values for activated sludge models were established. More importantly, a specialized microbial population may develop that will use the added carbon source with different kinetics than the wastewater COD that is degraded by traditional heterotrophs (Torres et al., 2011). This may require extension of the model structure. A critical evaluation of the applicability of default model parameters is always required, and such evaluation may sometimes suggest kinetic testing. For characterization of denitrification kinetics again, bioassays and simulation of full-scale data can be used.

3.2.1 *Bioassay Methods*

The parameter eta (η) that characterizes the reduction in rate under anoxic vs aerobic conditions can be estimated by comparing the oxygen utilization rate (OUR) (r_O) and the nitrate utilization rate (NUR) (r_{NO3}) in aerobic and anoxic batch tests using the same mixed liquor and organic substrate (Kristensen et al., 1992), as follows:

$$\eta = 2.86 \frac{r_{NO3,ex}}{r_{O,ex}} \tag{5.3}$$

The subscript "ex" refers to the exogenous rate, that is, the substrate-induced rate that is calculated by subtracting the endogenous rate from the overall r_O and r_{NO3} data (see Section 2.0 in this chapter).

The OUR is determined by monitoring the decrease of dissolved oxygen following the addition of a readily biodegradable substrate, such as acetate. The NUR is determined by measuring the nitrate decrease when adding the same organic substrate (e.g., acetate) to mixed liquor under anoxic conditions (no oxygen, only nitrate present). Details for these tests can be found in work by Melcer et al. (2003). An example of high-frequency NUR and OUR data collected using nitrate and dissolved oxygen sensors in a batch setup is given in Figure 5.4.

3.2.2 *Simulation of Full-Scale Dynamic Behavior*

Effluent or in-process nitrate concentration data can be used as a target variable to calibrate the denitrification kinetics parameters, the latter of which typically are more information-rich and leads to more reliable estimates. It is important to ensure that the correct amount of organic substrate is being made available to the denitrifiers

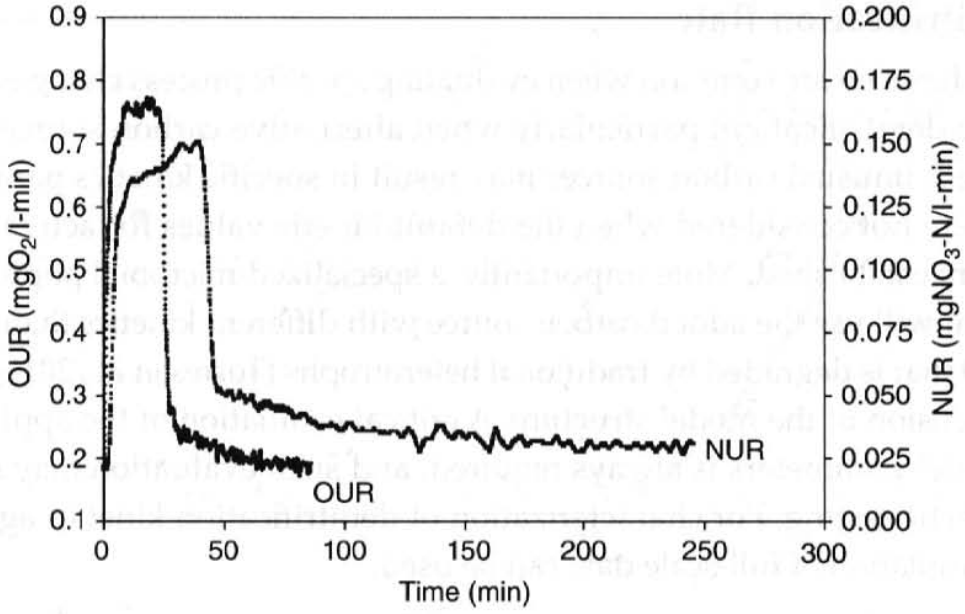

FIGURE 5.4 Comparison of acetate-based OUR (47 mg COD/L acetate added) and NUR (39 mg COD/L acetate added) determinations using dissolved oxygen and nitrate sensors in a batch setup. Note the endogenous respiration rate (0.2 mg O_2/L·min; 0.03 mg NO_3-N/L·min) that needs to be subtracted to obtain the exogenous rates required for the kinetic parameter. (Sin and Vanrolleghem, 2004).

during the simulation. This means that the influent composition (see Section 2.0) and hydrolysis/fermentation parameters (e.g., with methods proposed by Kappeler and Gujer [1992]) must be determined beforehand.

4.0 HYDRAULIC CHARACTERIZATION

As explained in Section 3.1.4 of Chapter 2, practical mixing behavior in reactors can be modeled in two ways. Either the advection-dispersion equation is used, leading to the use of a partial differential equation that requires specific solvers that are computationally slow. The alternative approach that has been adopted in the wastewater industry is based on a discretization of the spatial dimension. This results in the tanks-in-series model (Gujer, 2009).

The following approaches can be used to determine the number of tanks-in-series to be used: the empirical equation approach and an experimental approach based on tracer testing. These are briefly introduced in the following section.

4.1 Empirical Equation Approaches

Chambers and Jones (1988) at WRc plc (Swindon, U.K.) developed the following simple empirical relationship between the number of tanks-in-series (N) and the geometry and flow-through rate of a reactor:

$$N = 7.4\frac{L}{WH}Q_{in} \tag{5.4}$$

where

N = the number of tanks-in-series describing the mixing regime of the reactor (-)

W, H, and L = the dimensions of the tank (i.e., width, height, length [m])

Q_{in} = the flowrate through the tank (m^3/s)

For large facility-wide models or complex submodels, this formula may result in an overly complex model layout. The modeler should always use common sense when balancing model complexity with the model objective. If the formula recommends 10 units in series to simulate an aeration basin but the modeler knows that there are only five different diffuser grid types, it may be sufficient to include only five reactors in series. On the other hand, if a square anoxic zone is partitioned with three baffle walls, it may be important to include three reactors in series to simulate the plug flow pattern. Model calibration and validation efforts will confirm whether what the modeler has developed included the appropriate level of complexity.

An alternative, more accurate (but also more complex) empirical equation was proposed by Fujie et al. (1983). It analyzes the number of tanks describing a reactor zone, using the Peclet number, Pe, as follows:

$$N = \frac{Pe^2}{2}(Pe - 1 + e^{-Pe}) \tag{5.5}$$

With $Pe = \frac{\mu L}{E_L}$ (-) with u the average velocity (cm/s), L the zone length of the reactor (cm), and E_L the longitudinal dispersion coefficient (cm^2/s) that is calculated as follows:

$$E_L = 0{,}0115\left(1 + \frac{H}{L}\right)^{-3} \mu_g^{-0.34} a_d \Phi^{m_d} (H + W) \tag{5.6}$$

$$\Phi = h u_g \left(\frac{h}{H}\right)^{1/2} \left(\frac{H}{W}\right)^{1/3} \tag{5.7}$$

TABLE 5.2 Values of Fujie empirical constants a_d and m_d as a function of diffuser type and Φ as specified in Eq. 5.7.

Type of air diffuser	Φ(cm²/s)	m_d	a_d
Fine bubble types[a]	$\Phi \leq 20$	0.64	7.0
	$\Phi > 20$	0.46	12.0
Coarse bubble types[b]	$\Phi \leq 20$	0.78	3.5
	$\Phi > 20$	0.56	4.9

[a]Porous plates and tubes.
[b]Perforated plates and tubes, single nozzles, and others.

where

H and W = the height and width (cm) of the reactor zone, respectively
u_g = superficial gas velocity (cm/s) calculated from the airflow rate and the zone surface area
h = diffuser depth (cm)
a_d and m_d = Fujie empirical constants that can be read from Table 5.2

Makinia and Wells (2005) reported that Fujie's equation gives satisfactory results for most standard cases. A spreadsheet with these two estimation formulae is provided by Rieger et al. (2012).

4.2 Tracer Testing

An experimental approach to determine the number of tanks describing the mixing regime of a reactor is to perform an experimental tracer study by injecting a pulse of an inert tracer or to increase its concentration for a prolonged period at the reactor inlet. The inert nature of the tracer is important because the substance should not adsorb to the sludge and should not be degraded. To verify this, a mass balance should be made to ensure that all tracers have been recovered by the end of the tracer experiment. The time series of recovered tracers is then measured at the outlet of the reactor under study. Although this experimental approach is more time-consuming and expensive, it is more accurate. It is important to note that this does not account for any wet weather flow, unless the tracer test is repeated with different inflow rate conditions. Another significant effect on mixing behavior is caused by aeration. High aeration intensity typically leads to increased mixing and, therefore, to less plug flow behavior (modeled as fewer tanks in series).

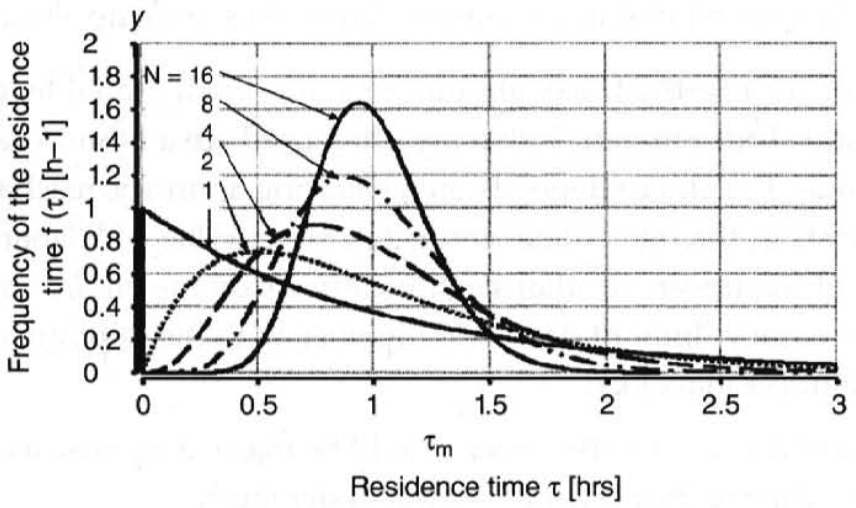

FIGURE 5.5 Ilustration of the effect of a different number (N) of continuously stirred tank reactors in series to describe mixing behavior. The y axis represents RTD and τ_m represents the dimensionless time based on the mean residence time in all N tanks.

Typical model-based responses to tracer injections are given in Levenspiel (1999). The pulse injection case is reproduced in Figure 5.5, and similar figures can be found for the step change experiment (the reader should note that a step is the integral of a pulse and that, because of linear system equations, step responses are the integrals of the pulse responses). When performing experiments, recycle flows typically present in WRRFs can complicate the interpretation. To allow for the simple interpretation of tracer test data, recycling could be switched off. In such instances, simple calculations allow finding the number of tanks-in-series from the data (Gujer, 2009).

In instances where more complicated flow patterns are observed (short-circuiting, recycles), an approach using simulation models with different configurations of tanks and recycles can be simulated in a facility simulator (using an inert soluble component as a surrogate for the tracer). The best-fitting model determines the configuration of tanks to be used subsequently. Figure 5.5 shows that using one tank gives rise to the typical exponential decay model response of an ideally mixed tank. Increasing the number of tanks results in the buildup of a peak, which becomes higher in absolute value and whose occurrence is shifted further in time. This is the typical behavior of a complete plug flow system. When the number of tanks reaches infinity, a perfect plug flow response is approximated, that is, all tracer appears at once at the outlet after a time corresponding to hydraulic residence time (HRT).

The following procedures are recommended when setting up a tracer experiment:

- Choice of tracer—the tracer should be a non-biodegradable, non-adsorbing compound. Tracer materials that are often used are a lithium salt, rhodamine, or bromide. The choice depends on measuring accuracy, reachable measuring frequency (e.g., through online sensors or only possible with laboratory analysis), toxicity of the tracer, or other negative effects on the environment. The measuring accuracy/limit of detection together with the flowrate determines the required tracer mass load.
- Injection of the tracer—the tracer should be injected as close as possible to the entrance of the reactor/facility section under study.
- Data collection—samples should be taken as close as possible to the exit of the reactor under study. Samples should be collected for a period that covers at least three to five HRTs. During this period, about 20 to 50 samples should be taken. If possible, a first screening of tracer dynamics should be conducted and only samples taken at times where the highest variations are visible should be analyzed further if the budget is limited. Considering Figure 5.5 and the typical mixing regime in bioreactors (three to 10 tanks-in-series), most samples should be taken before HRT is reached, with some samples taken to monitor the tailing. It may also be useful to wait until the recycle kicks in (i.e., until the tracer comes back with the recycle flows). While these additional dynamics complicate interpretation, they give valuable information.

An example of a tracer test performed at full scale is shown in Figure 5.6 (De Clercq et al., 1999). In this example, it was observed that using one tank is not sufficient to model the mixing behavior. However, when using two tanks-in-series, the performance of the model is satisfactory.

Flow splitting also deserves attention when modeling WRRFs. Splitting chambers are typically modeled as ideal flow splitters. However, in reality, this is often not the case, and this can have a large effect on modeling results. One way to investigate an influent splitting work is to investigate the sludge concentrations that occur in the different lanes. Theoretically, these should be the same when an equal loading is provided. The respective sludge concentrations in the different lanes for the aforementioned example are given in Figure 5.7. In terms of equal flow distribution, a line through the origin with a 45-deg slope should be found. Figure 5.7 shows that this is the case for lanes AS1 and AS3. However, lane AS2 exhibits a much larger sludge

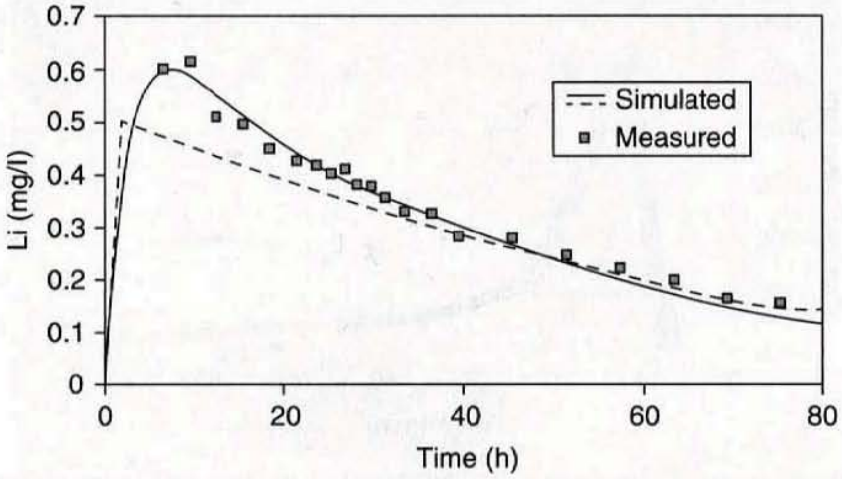

FIGURE 5.6 Illustration of model fits to RTDs in train 1 recorded using Lithium as tracer, with one tank (dashed line) and two tanks in series (solid line). Note the bump on the graph at approximately 35 hours caused by recycle of tracer.

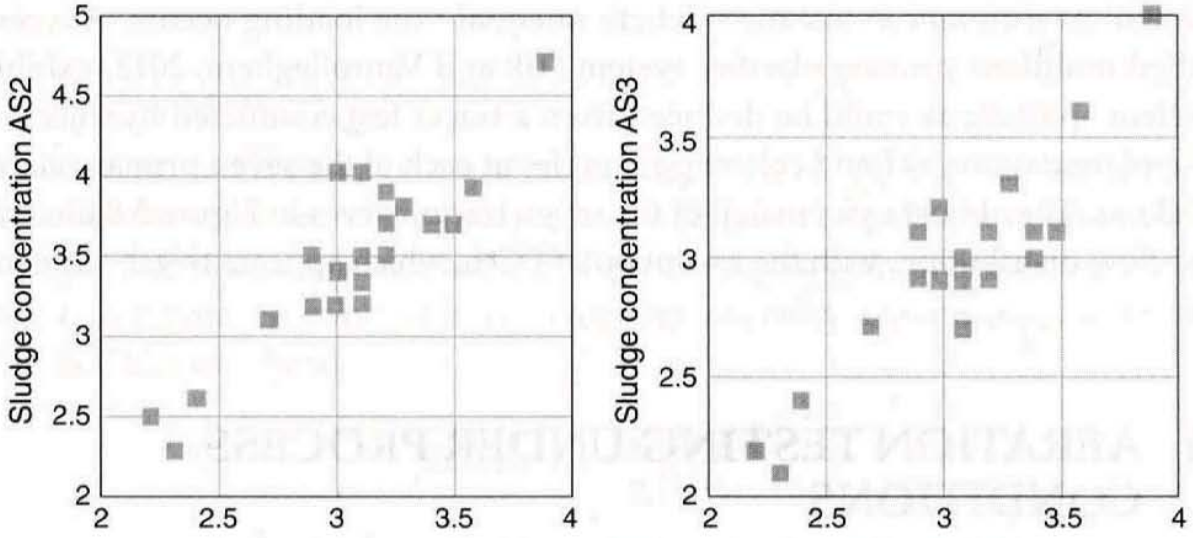

FIGURE 5.7 Illustration of differences in sludge concentration in different lanes caused by an improperly functioning flow-splitting works.

concentration (+20%), suggesting that more sludge and less wastewater is going to that lane, leading to a loss in treatment performance. Closer investigation of the influent splitting works revealed shortcut flows of both the influent and return activated sludge (RAS) from the secondary settlers.

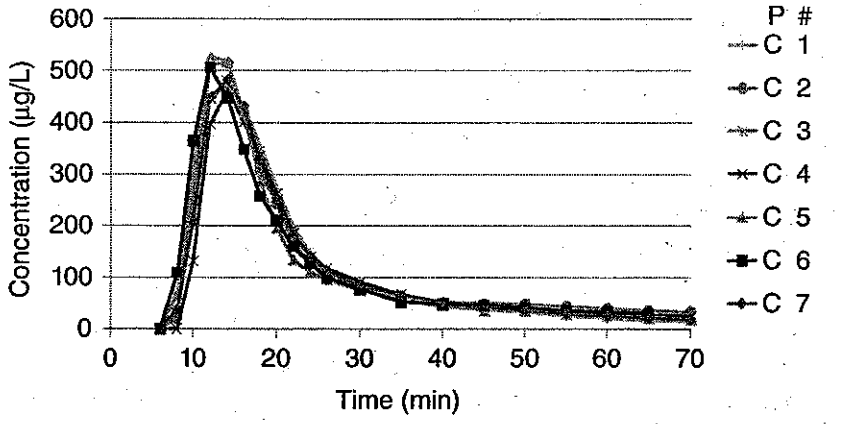

FIGURE 5.8 Illustration of rhodamine wastewater treatment tracer test results for detection of unequal flow splitting in a multilane primary clarifier system. (Tik and Vanrolleghem, 2012).

A tracer study can also be used to identify unequal flow splitting. The residence time will be different in instances where unequal flow loading occurs. A recently studied multilane primary clarifier system (Tik and Vanrolleghem, 2012) exhibited excellent splitting as could be deduced from a tracer test conducted by injecting a pulse of rhodamine WT and collecting samples at each of the seven primary clarifier overflows. The almost exact match of the seven tracer curves in Figure 5.8 illustrates good flow distribution, with the exception of PC#6, which appears to get some more load.

5.0 AERATION TESTING UNDER PROCESS CONDITIONS

The performances of aeration systems in WRRFs are typically guaranteed and measured in clean water according to a standardized method, the unsteady-state clean water test (ASCE, 2007). Translation from clean water conditions to process conditions requires determination of the alpha factor, which depends on many parameters (see Chapter 8). Oxygen transfer rates can also be characterized under process conditions using several methods (ASCE, 1997; Capela et al., 2004). The following two methods, in particular, can be applied: the offgas analysis method developed by Redmon et al. (1983) and the hydrogen peroxide method originally proposed by Kayser (1979).

FIGURE 5.9 Sampling hood. (Credit: Y. Fayolle, Irstea).

5.1 Offgas Method

The offgas method is based on a gas-phase mass balance. The gas bubbles at the liquid surface are collected using floating hoods (Figure 5.9). At each hood location i, the offgas flowrate ($q_{e,i}$) is measured and the molar oxygen concentration is determined to compute the standard oxygen-transfer efficiency under process water (field SOTE, $SOTE_{f,i}$), as follows:

$$SOTE_{f,i} = 1 - \frac{y_s(1-y_e)}{y_e(1-y_s)} \tag{5.8}$$

where y_e, y_s is the molar oxygen concentration in the insufflated air and in the offgas (-).

The overall $SOTE_f$ of the aeration system is obtained by weighting the $SOTE_f$ values by the offgas flowrates collected at each test location, as follows:

$$SOTE_f = \frac{\Sigma q_{e,i} \times SOTE_{f,i}}{\Sigma q_{e,i}} \tag{5.9}$$

Full-scale aeration testing using the offgas method requires prior definition of a representative gas-sampling plan such as that exemplified in Figure 5.10.

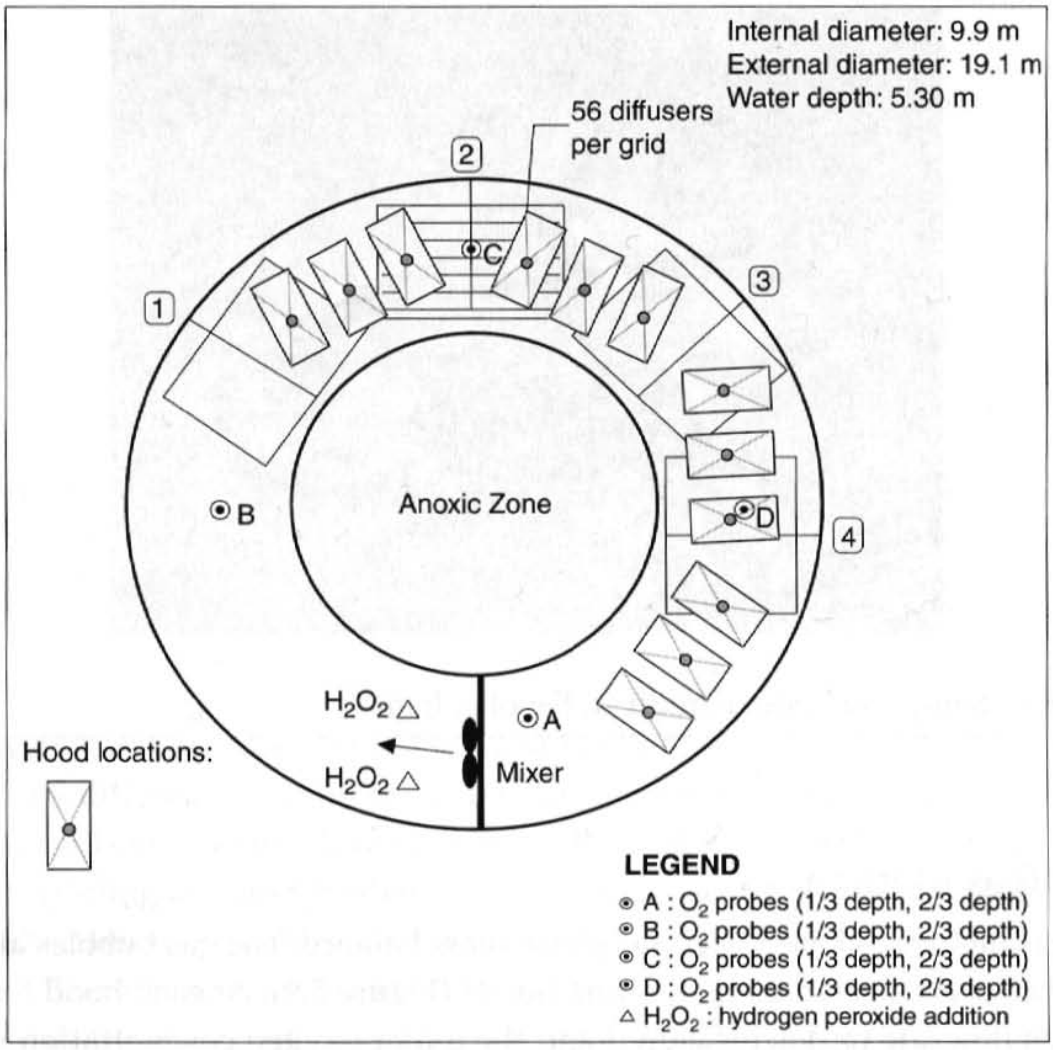

FIGURE 5.10 Illustration of an offgas sampling plan. (Credit: Capela et al. [2004]).

Gas-sampling plans vary from one facility to another depending on the geometry of the tank and the distribution pattern of the aeration system.

5.2 Hydrogen Peroxide Method

The hydrogen peroxide method allows the determination of $k_L a_f$ by monitoring the dissolved oxygen concentration over time after adding hydrogen peroxide (H_2O_2) to create a perturbation from steady-state conditions. The dissolved oxygen concentration during the deaeration period can be written as follows (ASCE, 1997):

$$C = C_R - (C_R - C_0) \times e^{-(k_L a_f + Q/V)xt} \tag{5.10}$$

where

C = actual dissolved oxygen concentration (mg/L)
C_R = the concentration at steady state in process water (mg/L)
C_0 = initial dissolved oxygen concentration (mg/L)
$k_L a_f$ = volumetric mass-transfer coefficient in process water ($1/T$)
Q = volumetric wastewater flowrate (m^3/h)
V = tank volume (m^3)

The addition of H_2O_2 is performed maintaining a constant power level. The goal is an increase in the dissolved oxygen concentration above the steady-state dissolved oxygen concentration (C_R) higher than 10 mg/L. For a 35% H_2O_2 solution, the volume to inject is determined as follows:

$$V_{H_2O_2,35\%} = 5,37\Delta CV10^{-6} \tag{5.11}$$

where

$V_{H_2O_2,35\%}$ = volume of peroxide solution (35%) to inject (L)
ΔC = increase in dissolved oxygen concentration (mg/L)
V = tank volume (L)

An example of a deaeration curve is presented in Figure 5.11.

6.0 SLUDGE SETTLING CHARACTERIZATION

A detailed settling characterization is necessary if the settling performance and the reactions during settling influence overall system behavior (e.g., effluent COD, nitrogen, and phosphorus). In addition, the target(s) might be the optimization of settling or may be the amendment of effluent suspended solids (ESS) removal. Hindered and compression settling are the main phenomena taking place in secondary settlers. Primary settlers that are characterized by discrete and flocculation-type settling are discussed at the end of this section.

In addition to the sedimentation process, reactions such as denitrification (leading to gas-bubble formation that disturbs settling) and phosphorus release in the settler may have to be considered (Henze et al., 1993; Koch et al., 1999; Wouters-Wasiak et al., 1996). This can be checked by calculating the mass balance over nitrate-phosphate or by site observations such as the occurrence of nitrogen gas bubbles trapped in the flocs (Henze et al., 1993). Information on flow velocity measurements is given at the end. They are of special interest when carrying out a detailed evaluation of clarifiers using computational fluid dynamics (CFD) models.

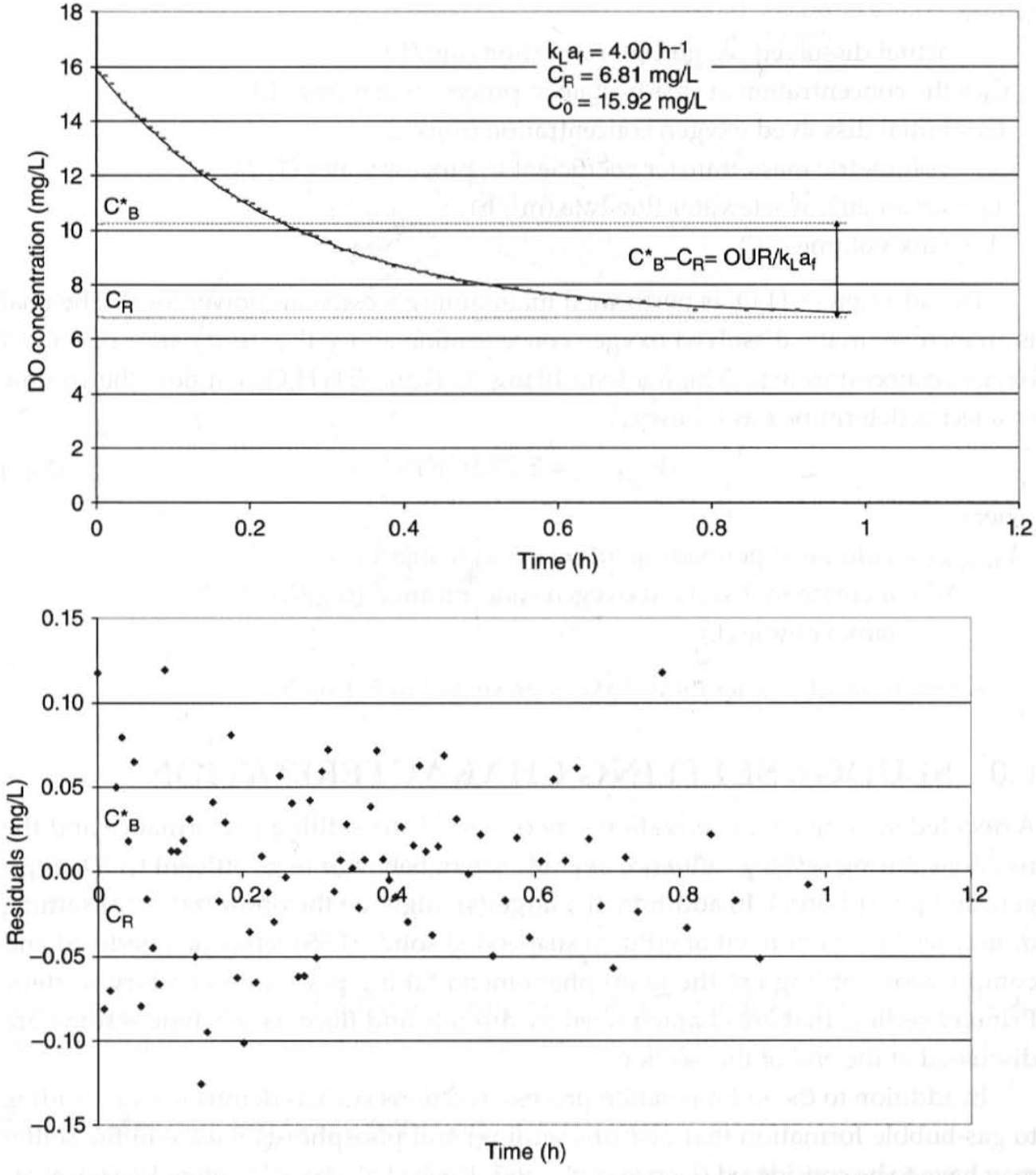

FIGURE 5.11 Dissolved oxygen concentration (top) and residuals (bottom) during a deaeration test after the addition of hydrogen peroxide.

6.1 Full-Scale Tests

Estimation of a settler model's parameters can be performed by fitting the model outputs to time series of flowrates and total suspended solids (TSS) concentrations measured at the clarifier's inlet, underflow, and effluent. The latter data can either be obtained by offline TSS measurements or by turbidity sensors. Provided they are properly handled, the latter have reached a level of reliability and precision that allows their use for model calibration (Vanrolleghem and Lee, 2003). It is important to realize that best calibration performance will be obtained under dynamic conditions because these better expose the dynamics of the settler.

For more advanced models, it may be necessary to supply data taken within the clarifier. Turbidity sensors that move up and down in the clarifier or ultrasonic profilers may provide time series of the sludge blanket height and even sludge profiles (Figure 5.12).

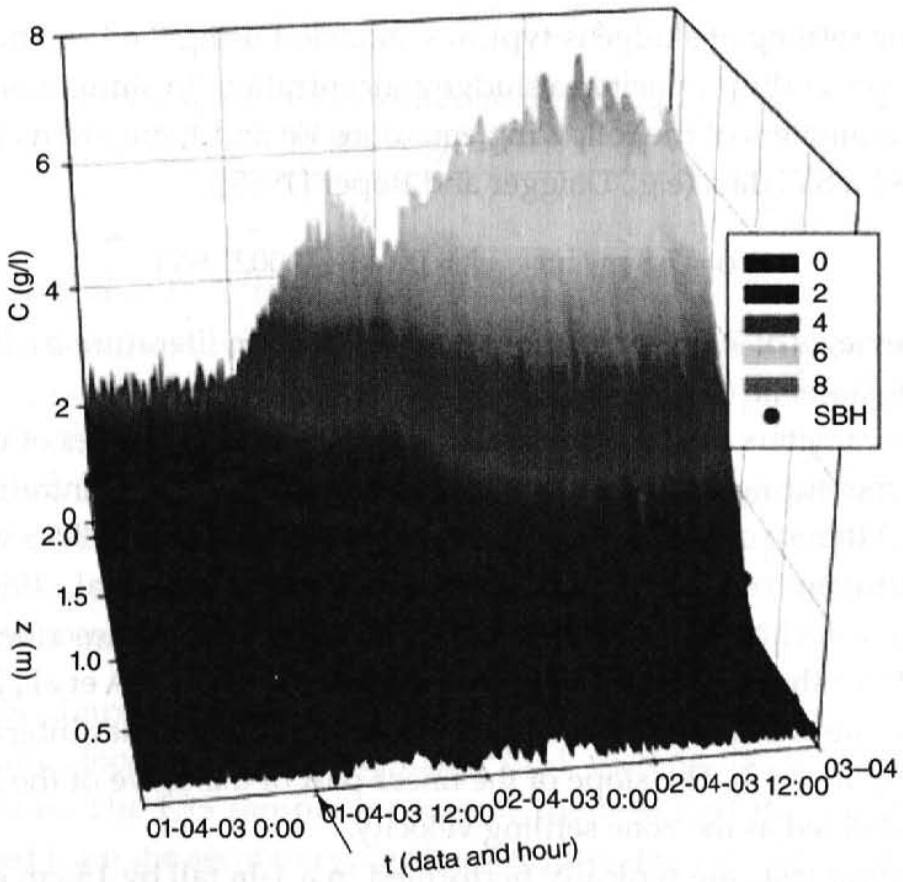

FIGURE 5.12 Sludge concentration profiles and sludge blanket height (SBH) during stress testing a secondary clarifier at the Heist water resource recovery facility. (De Clercq, 2006).

Highly informative data sets, in particular, can be obtained from clarifier stress tests (Wahlberg, 2002) that involve hydraulically stressing an existing final clarifier such that the dynamic clarifier performance may be monitored in effluent and underflow. This is achieved by taking units offline until the targeted surface overflow rate (SOR) and solids loading rates (SLRs) are reached. Operating performance is continuously monitored until performance reaches a determined "failure" point, such as high effluent TSS or high blanket level, at which point the stress testing is ended and the offline units are returned to service. Parameters monitored for each operating clarifier include sludge blanket levels, mixed liquor suspended solids, ESS, RAS, TSS, sludge volume index (SVI), flowrates, dispersed suspended solids (DSS), and flocculated suspended solids (FSS).

6.2 Laboratory Testing

6.2.1 Hindered Settling Parameters

Hindered zone settling of sludge is typically modeled using the Vesilind equation or alike that relates settling velocity to sludge concentration. In simulation studies, the two kinetic parameters of the following equation, V_o and k, are often obtained from correlations with SVI data (e.g., Daigger and Roper [1985]):

$$V_o = 7.8 \text{ m/h}; \qquad k = 0.148 + 0.0021 \text{ SVI}$$

Critical reviews of such correlations can be found in literature by Bye and Dold (1999) and Giokas et al. (2003).

Settling parameters can be determined directly by using a series of batch column settling tests, measuring settling velocities at different sludge concentrations (Bye and Dold, 1999). Different concentrations are obtained by dilution of RAS with effluent. At least six different concentrations should be tested (Ekama et al., 1997). The individual settling velocities are measured following the procedure described in *Standard Method* 2710 E for the evaluation of the zone settling rate (APHA et al., 2005), that is, the descent of the sludge–water interface is monitored at regular intervals for 30 to 60 minutes (Figure 5.13). The slope of the linear part of the curve of the interface displacement is defined as the zone settling velocity.

Batch settling tests are typically performed in a 1-m tall by 15-cm diameter settling column provided with a stirring mechanism to minimize wall effects. Automated systems that can be installed in the field for online characterization of settling performance have been developed (Vanrolleghem et al., 2006).

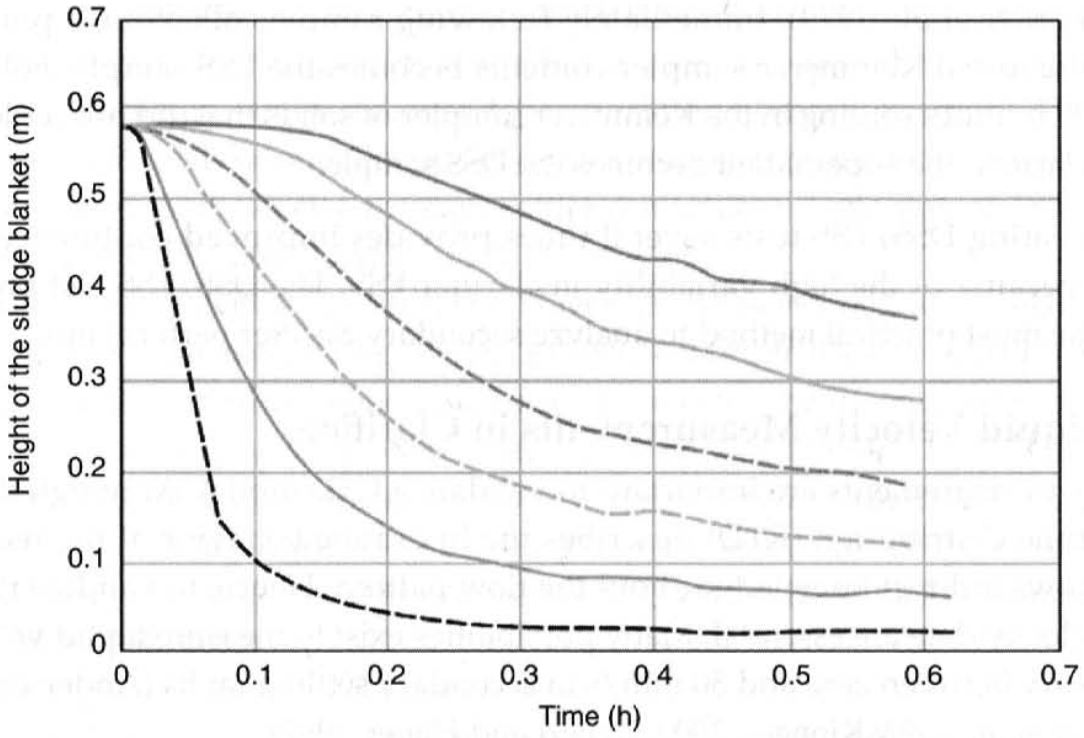

FIGURE 5.13 Batch settling curves for different initial sludge concentrations (from bottom to top: 3, 5, 7.7, 9.7, 12.7, and 15.6 g/L).

6.2.2 *Nonsettleable Fraction*

The nonsettleable fraction of the suspended solids, f_{ns}, can readily be measured in a settling column analysis (Takács et al., 1991) or, as mentioned previously, from a time series of effluent TSS measurements.

To gain more insight to the ultimate settleability of suspended solids, the DSS/FSS test can be conducted (Ekama et al., 1997; Wahlberg, 2002). Conducting the DSS/FSS test requires measurement of TSS in three samples, two of which must be collected in a special manner, as follows:

- The FSS sample consists of supernatant from a settled mixed liquor sample following flocculation in a standard 2.0-L rectangular beaker flocculation apparatus. The FSS sample represents the best performance (lowest ESS) expected from the secondary clarifier because, theoretically, ideal flocculation and settling occurred prior to sampling the supernatant.
- The DSS sample consists of secondary clarifier effluent collected using a modified Kemmerer sampler at the clarifier effluent weir (Ekama et al., 1997;

Parker et al., 1970). Immediately following sample collection, a portion of the initial Kemmerer sampler contents becomes the ESS sample. Following 30 minutes settling in the Kemmerer sampler of solids that did not settle in the clarifier, the supernatant becomes the DSS sample.

Repeating DSS/FSS tests several times provides improved confidence in the results because of the high variability in clarifier ESS. The DSS/FSS test presently offers the most practical method to analyze secondary clarifier performance.

6.3 Liquid Velocity Measurements in Clarifiers

Velocity measurements are important to validate a CFD model. Although the residence time distribution (RTD) describes the hydraulic behavior of the reactor, it only allows indirect knowledge about the flow pattern. Hence, to validate the flow field, velocity data are essential. Many possibilities exist to measure liquid velocities, which vary between zero and 80 mm/s in secondary settling tanks (Anderson, 1945; Bretscher et al., 1992; Kinnear, 2000; Ueberl and Hager, 1997).

The basic method proposed by Anderson (1945) is still in use, although other measurement techniques are available. These alternative flow velocity devices can be subdivided into the following three groups: mechanical (Lindeborg et al., 1996; STOWa, 2002a,b), electromagnetic, and acoustic Doppler velocity meters (Deininger et al., 1998; Kinnear and Deines, 2001). Whereas the former two techniques measure true liquid velocity, the acoustic Doppler velocity meter measures the velocity of small particles suspended in the liquid.

6.4 Primary Clarifiers

Attention to primary clarifier modeling has been lacking in wastewater treatment modeling for a long time. Often, modeling only started with primary effluent. However, increased attention on energy-neutral WRRFs and the role primary clarifier performance plays in this has put this unit process back in the spotlight (Crawford et al., 2010).

Current primary clarifier models describe settling according to Stokes' law, even though flocculent settling conditions may occur. The latter process warrants analysis and inclusion in the model description, especially in chemically enhanced primary clarifiers. While analysis using coagulation/flocculation tests is well established (Melcer et al., 2010), the models are not really applied and the effect of chemical addition is simply included as an improved separation efficiency or higher settling velocity.

The parameters of primary clarifier models are typically deduced from inlet–outlet TSS-removal performance analysis (e.g., Lessard and Beck, 1988) or batch settling experiments conducted over different settling times (Otterpohl, 1995). The settleable solids analysis after 2 hours of sedimentation gives a good indication of the maximal removal efficiency a primary settler can achieve. Supernatant TSS concentrations indicate the nonsettleable solids.

Recently, more detailed experimental methods are developed to characterize settling in primary clarifiers. Using the ViCAs protocol originally developed for stormwater characterization (Chebbo and Gromaire, 2009), the distribution of settling velocities of raw and clarified wastewater can be obtained (Figure 5.14) (Maruejouls et al., 2011). From such graphs, it is easy to deduce which mass fraction will be removed by a primary clarifier, and models that use settling velocity classes of particles are currently being developed to better describe the dynamics of primary clarifiers (Bachis et al., 2012).

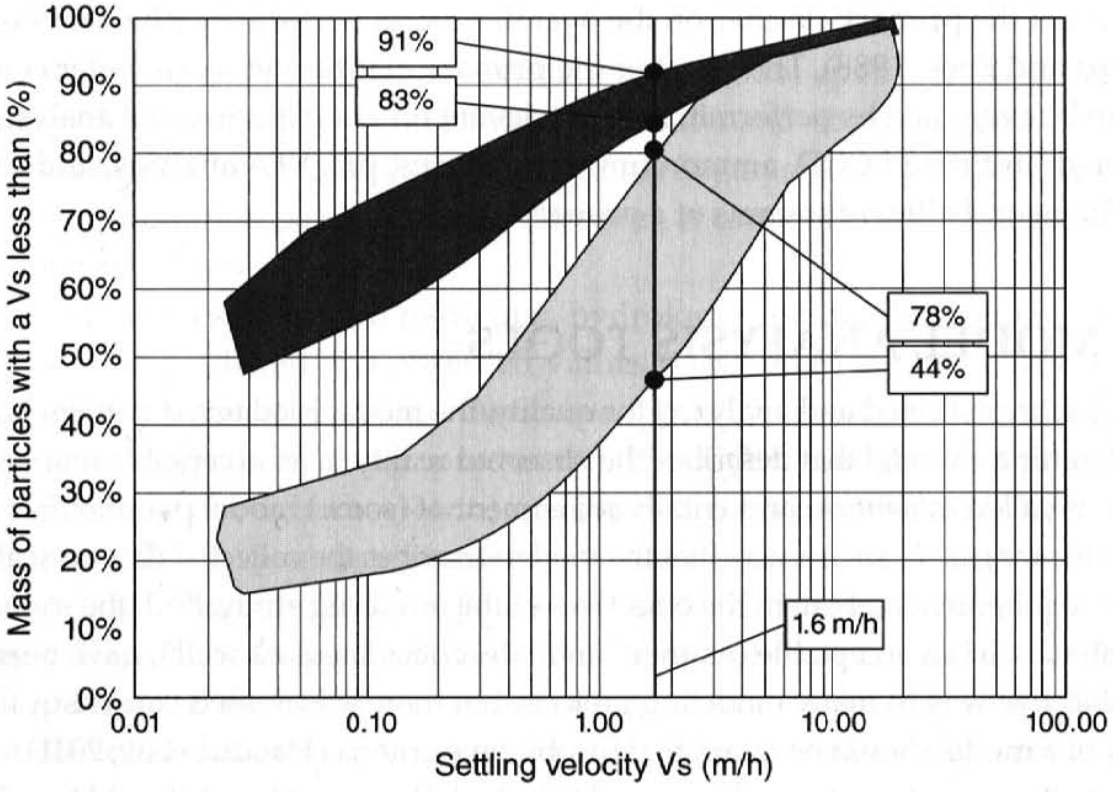

FIGURE 5.14 Settling velocity (Vs) distribution curves for dry weather wastewater. "Dark" is the Vs distribution range of wastewaters from the effluent of primary settling. "Pale" is the Vs distribution range of wastewaters from the influent of primary settling. (Maruejouls et al., 2011).

A ViCAs curve must be interpreted as follows: the lower the curve the larger the fraction of rapidly settling particles. Considering a sedimentation velocity of 1.6 m/h to be the typical design overflow rate for primary sedimentation units (Metcalf and Eddy, 2003), Figure 5.14 shows that between 83% and 91% of the particle masses at the outlet of the primary settler have a settling velocity lower than their design value (1.6 m/h). Furthermore, between 44% and 78% of the influent particle masses have settling velocities lower than 1.6 m/h, resulting in 56% to 22% of particle masses that can be intercepted by a primary settler.

The primary clarifiers ahead of the biological reactors also have a vital importance because there might be activation and/or interactions between physico-chemical and biological reactions. For instance, in addition to biological reactions, COD removal can be expressed as a physico-chemical reaction such as flocculation and solubilization of the particulate COD fractions into soluble fractions. The biomass in wastewater also induces biological processes such as fermentation, acidification, and ammonification. The settling and biological reactions should, therefore, be combined in the model if the effect of the primary clarifier on the overall process performance becomes evident (Lessard and Beck, 1988). The effect of the primary clarifier on wastewater composition can be evaluated by performing some relevant on-site experimental analyses such as filtered/unfiltered COD, ammonium, phosphorus, pH, VFA analysis, and so on in the influent and effluent streams of a primary clarifier.

7.0 MODEL ANALYSIS TOOLS

After data are collected and analyzed for quality, the model is adjusted to them with the goal of getting a model that describes the observed reality in an acceptable manner. This activity is called *calibration*, and entails adjustment of (some) model parameters (within reasonable ranges) in such a way that the model describes the collected data well and fulfills the requirements set out in the objectives of the modeling study. Both the statements, "describes ... in an acceptable manner" and "describes the data well", have been used in a subjective way in many modeling projects, but there is increased consensus that the quality of a model should be quantified by objective criteria (Hauduc et al., 2011).

Not all parameters of a facility model (of which there are many) should be adjusted during calibration. Some authors even state that, for municipal WRRFs, no adjustment of kinetic and stoichiometric parameters is needed as the model with default parameters provides a prediction performance that is sufficient for the model purpose at hand. In most model applications, however, some model adjustment is required.

Some model parameters may obtain their value directly from some of the aforementioned dedicated experiments (e.g., settling properties, growth rates, and wastewater fractions), although these values could best be considered good initial estimates for further calibration steps given the issues with transferability of dedicated experiments to full-scale behavior (Gernaey et al., 2004; Petersen et al., 2003). For the remaining, often large number of parameters, there is often insufficient data available to obtain good estimates for all of them (i.e., the information content of the data set is insufficient to practically identify all parameters). Optimal design of experiments is one solution to this identifiability problem, yielding data that lead to better estimates of parameters (Vanrolleghem et al., 1995).

In general, however, resources are not available to estimate all parameters and, therefore, one is content with estimating those parameters that make a difference with respect to the quality of the model's predictions. Sensitivity and uncertainty analysis methods allow dealing with this and are discussed in Sections 7.3 and 7.4.

7.1 Goodness-of-Fit

In wastewater treatment modeling, evaluation of model quality is often based on qualitative comparisons between simulation results and observed data. Although such visual evaluation is useful, it does not provide an objective assessment of the quality of a calibration parameter set. Moreover, it cannot be used in an automatic calibration procedure.

Environmental sciences (in particular, hydrology) commonly use mathematical comparisons of predicted and observed values (Dawson et al., 2007). In wastewater treatment, several target constituents are typically considered simultaneously during model calibration (sludge production, TSS, COD, nitrogen, and phosphorus in the effluent). Although a review of quality criteria is presented in Dochain and Vanrolleghem (2001), quantitative criteria are rarely determined in wastewater treatment modeling (Ahnert et al., 2007; Petersen et al., 2002; Sin et al., 2008).

Depending on modeling objectives, the goodness-of-fit of a model can be defined as the capability of the model to capture one or several of the following characteristics of observed data: mean, timing, and magnitude of peaks or typical periodical variations (diurnal, weekly, seasonal, etc.). For example, if a specific effluent limit of a facility is based on a monthly average, there is little sense in evaluating the accuracy of the fit of each single peak. However, if peak effluent limits have to be met, a criterion evaluating the fit of peaks should be used. Thus, to characterize the goodness-of-fit of the model, different quality criteria may be needed.

Hauduc et al. (2011) selected 31 quantitative goodness-of-fit criteria in a comprehensive literature review. They were grouped according to two classification systems. The first classification scheme is inspired by Dawson et al. (2007) and groups the criteria into the following six main classes:

1. Single event statistics—in instances where modeling objectives require accurate simulation of events (e.g., the ability of the WRRF to handle storm flows or toxic peaks), criteria are needed to characterize the goodness-of-fit of the model for this event. The goal of the single-event statistics peak difference (Gupta et al., 1998) and percent error in peak (Dawson et al., 2007) is to characterize the difference between the maximum observed and maximum modeled value.
2. Absolute criteria from residuals—absolute criteria are based on the sum of residuals (difference between observed O_i and predicted P_i values, respectively, at time step i), generally averaged by the number of data, n. A low value of this criterion means good agreement between observation and simulation (with γ an exponent).

$$E_\gamma = \frac{1}{n}\sum_{i=1}^{n}(O_i - P_i)^\gamma \tag{5.12}$$

3. Residuals relative to observed values—at each time step, error is related to the corresponding observed or modeled value. A low value of this criterion means good agreement between observation and simulation.

$$RE_\gamma = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{O_i - P_i}{O_i}\right)^\gamma \tag{5.13}$$

4. Total residuals relative to total observed values—for these criteria, the sum of errors is related to the sum of observed values, without any correspondence to the time step. A low value of this criterion means good agreement between observation and simulation.

$$TRE_\gamma = \frac{\sum_{i=1}^{n}(O_i - P_i)^\gamma}{\sum_{i=1}^{n}O_i^\gamma} \tag{5.14}$$

5. Agreement between distributional statistics of observed and modeled data—these criteria are not based on error comparison, but on a comparison between cumulative distributions of modeled and observed data. In the

wastewater field, these criteria can be relevant for influent and effluent pollutant loads by summing the fluxes.

6. Comparison of residuals with reference values and with other models—these criteria compare the residuals with residuals obtained with a reference model $\tilde{P}$, such as a model describing the mean value ($\tilde{P}_i = \bar{O}$) or the previous value ($\tilde{P}_i = O_{i-1}$) (with α an exponent).

$$CE_{\alpha,\gamma} = 1 - \frac{\sum_{i=1}^{n} (O_i^{\alpha} - P_i^{\alpha})^{\gamma}}{\sum_{i=1}^{n} (O_i^{\alpha} - \tilde{P}_i^{\alpha})^{\gamma}} \tag{5.15}$$

In a second classification system, Hauduc et al. (2011) classified the 31 quality criteria as six main characteristics of the adjustment of the predicted values to the observed data set. Indeed, the study showed that the criteria clustered in only six different types, each focusing on one of the following objectives:

1. Criteria evaluating the mean error
2. Criteria evaluating the bias
3. Criteria that emphasize large errors
4. Criteria that emphasize small errors
5. Criteria evaluating peak magnitudes
6. Criteria evaluating event dynamics

Strong correlations exist between the values obtained with members of the same cluster, indicating that there are redundant criteria that do not add anything to the model quality evaluation. On the contrary, the existence of redundant criteria confuses communication because two groups of modelers may use different criteria without realizing that they are pursuing the same modeling objective. In addition, experience with criteria is divided among members of the cluster, meaning that less is known about the criteria and the interpretation of the values they take.

7.2 Parameter Estimation

Parameter estimation consists of determining the "optimal" values of the parameters of a given model with the aid of measured data. Figure 5.15 presents a schematic of the basic idea behind parameter estimation.

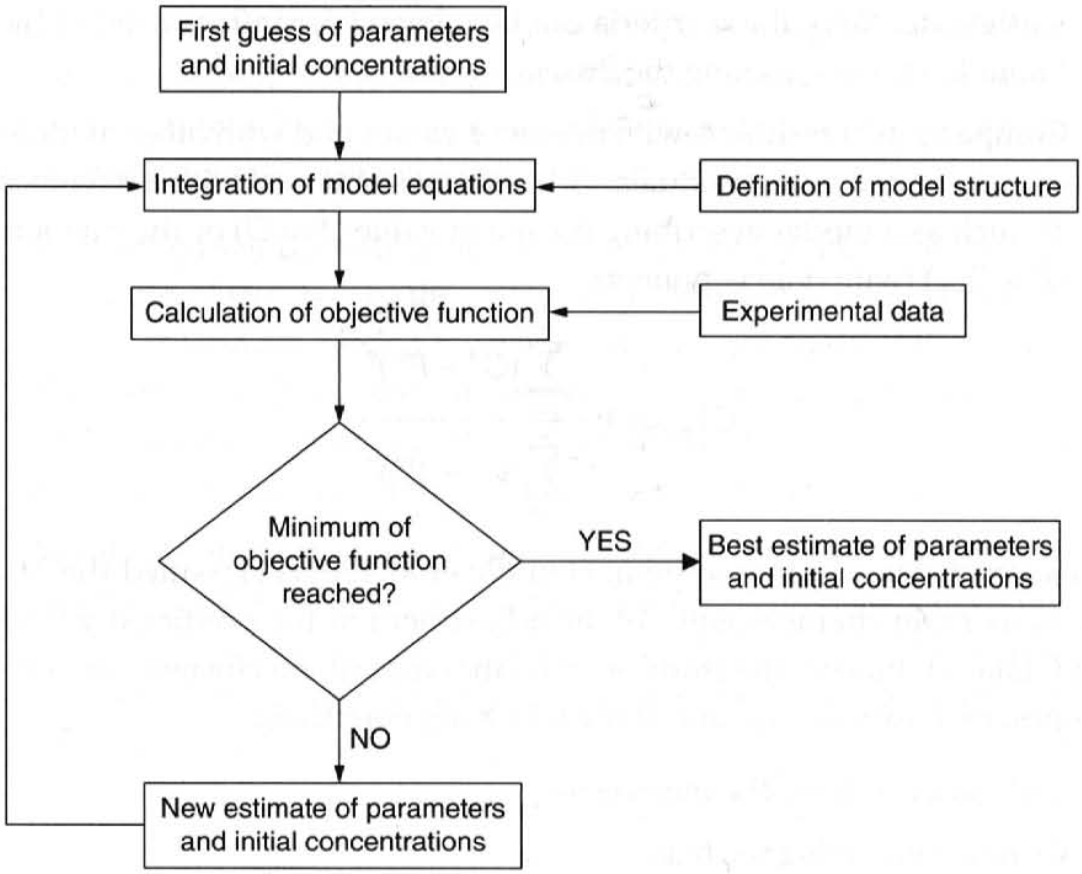

FIGURE 5.15 Illustration of parameter estimation routine. (Modified from Wanner et al. [1992]).

Initially, model structures, of which selected parameters need to be estimated, and experimental data need to be defined. Moreover, first guesses of the parameters to be estimated have to be given. The parameter estimation procedure then basically consists of minimizing an objective function J, which, for example, can be defined as the weighted sum of squared errors between the model output and data. When the objective function reaches a minimum with a certain given accuracy, optimal parameter values are obtained, as illustrated in Figure 5.16.

The modeler can conduct this search for the best parameter values in a trial-and-error manner until he or she finds a satisfying result for the quality criterion (it is important to keep track of the parameter sets already evaluated so that searches are not repeated). Other modelers use automated optimization algorithms. Although numerical techniques for automatic estimation will not be discussed here, the reader is referred to literature by Dochain and Vanrolleghem (2001).

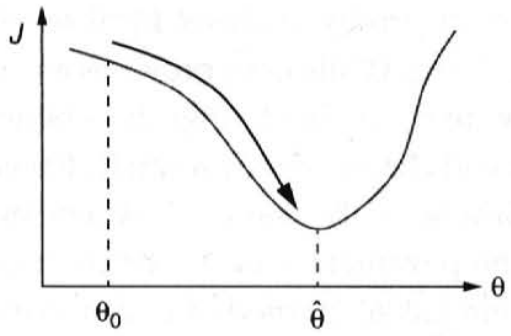

FIGURE 5.16 Minimization of a model quality criterion value J starting from an initial parameter estimate θ_0 to converge gradually (arrow) to the final, best estimate $\hat{\theta}$.

It is important to note, however, that because of the high complexity of the optimization problem caused by numerous parameters and the nonlinear nature of wastewater treatment models (Sin et al., 2008), it is cumbersome to apply automated calibration techniques. Rather, a combination of trial and error with intermittent use of an optimization algorithm is advised.

Indeed, a significant problem encountered in calibration of treatment models is the lack of identifiability of model parameters. *Identifiability* is the ability to obtain a unique combination of parameter values describing a system's behavior. This subject is dealt with in great detail in literature by Dochain and Vanrolleghem (2001). Here, it should only be stressed that a typical problem related to the calibration of wastewater models is that more than one combination of influent characteristics and model parameters can give the same good description of collected data (Dupont and Sinkjær, 1994; Kristensen et al., 1998). While this is acceptable for some model objectives (e.g., description of data), it is not for others (e.g., prediction for new situations as typically found in upgrade studies). In the latter instance, one must either reduce the number of parameters one can estimate (using expert knowledge or sensitivity analysis) or collect additional data to provide the information with which the parameter can be assessed.

7.3 Sensitivity Analysis

A sensitivity analysis studies the "sensitivity" of the outputs of a system (variables of interest) to changes in parameters. It also allows for ranking the model parameters according to how much they influence model outputs. Finally, a sensitivity analysis can be used to identify which model parameters can be estimated based on a given set of measurements. Only the most influential parameters will be retained for calibration.

There are two types of sensitivity analysis, local sensitivity analysis (LSA) and global sensitivity analysis (GSA). While GSA provides an "average" sensitivity of the nonlinear model outputs within a defined range of parameter values, LSA evaluates how much model outputs will change if only a small change is applied to the parameter values in the neighborhood of the assumed parameter values. Typical LSAs are carried out by altering the parameters by 1% of their assumed value, although De Pauw and Vanrolleghem (2006) warned of errors that occur when changes that are too large are applied.

A state-of-the-art LSA method for selecting parameters is one proposed by Brun et al. (2002). In this method, an overall sensitivity measure (δ) is calculated on the basis of scaled sensitivity values $s_{i,j}$ for each of the n model outputs i with respect to the parameters j:

$$\delta_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n} s_{i,j}^2} \tag{5.16}$$

$$s_{i,j} = \frac{\Delta p_j}{sc_i} \cdot \frac{\partial y_i}{\partial p_j} \tag{5.17}$$

where

Δp_j = the uncertainty range of the parameter p_j
sc_i = a scale factor
n = the number of model outputs considered

A large δ means that a change of Δp_j in parameter p_j has a substantial effect on the considered model output(s). Model parameters are typically assigned to three uncertainty classes according to Brun et al. (2002). Parameters from uncertainty class 1 (e.g., stoichiometry) have a low uncertainty (5% of the default parameter value); class 2 (growth rates) has an uncertainty range of 20% of the default parameter value; and 50% is recommended for parameters from uncertainty class 3 (e.g., half-saturation constants). Often-used scaling factors are (1) the model output value (or its average if a dynamic simulation is performed) or (2) the model output measurement error standard deviation. Ranking parameters on the basis of the δ_j values is the basis for selection of parameters to be estimated. Boltz et al. (2011) calculated δ_j for three bulk concentration predictions and four biofilm fluxes, respectively, at two different temperatures. It is important to note that the choice of output variables (i.e., expressing the interest of the modeler) determines which parameters are most influential and that temperature has a significant effect on δ_j values and ranking parameters in terms of importance for the model calibration.

With increasing available computing power, GSA methods are gaining in popularity as they can overcome the main problem of LSA, which is that LSA results are only valid for the parameter and input values used during the analysis. Because of the strongly nonlinear nature of the WRRF models, LSA results (e.g., the importance ranking of the parameters) are dependant on these factor values. Conversely, GSA methods assess how model outputs are influenced by the variation of the model input factors over their entire range of uncertainty (Saltelli et al., 2004). The GSA may help modelers select important factors ("factors prioritization") and noninfluential factors ("factors fixing") and identify interactions among factors. More specifically, by means of factors prioritization, model input factors that have the greatest effect on model outputs are identified. Conversely, the factors-fixing setting leads to the identification of factors that may be fixed at any given value over their uncertainty range without reducing the output variance (Saltelli et al., 2004).

The GSA is based on extensive simulation, typically using Monte Carlo simulation. Depending on the number of parameters to be considered and the GSA method used, hundreds to tens of thousands of simulations are required to adequately cover the entire range of uncertainty of the factors.

In Saltelli (2000), GSA methods are classified as (1) global screening methods (e.g., Morris screening method [Campolongo et al., 2007; Morris, 1991]); (2) variance decomposition methods such as Fourier amplitude sensitivity testing (FAST), extended-FAST (E-FAST), and the Sobol indices method (Saltelli et al., 1999; Sobol, 2001); and (3) regression/correlation-based methods such as the standardized regression coefficients (SRCs) method (Saltelli et al., 2008). Although it is beyond the scope of this chapter to explain in detail how these methods actually work, their interpretation and how they can be used in model parameter selection are relevant.

Mannina et al. (2012) suggest a common terminology on the basis of definitions drawn from literature by Saltelli (2000), Campolongo et al. (2007), and Pujol (2009). The first definition comes with the SRC method which, by defining a cutoff threshold (CFT), distinguishes between the following two factors (Figure 5.17a):

- Important factors—if sensitivity > CFT
- Nonimportant factors—if sensitivity < CFT

Important factors represent those model factors that have a high sensitivity coefficient and where, therefore, the modeler should pay more attention. Conversely, nonimportant factors are those model factors characterized by a low sensitivity coefficient. Linear models can be fixed anywhere in their variation ranges. For nonlinear

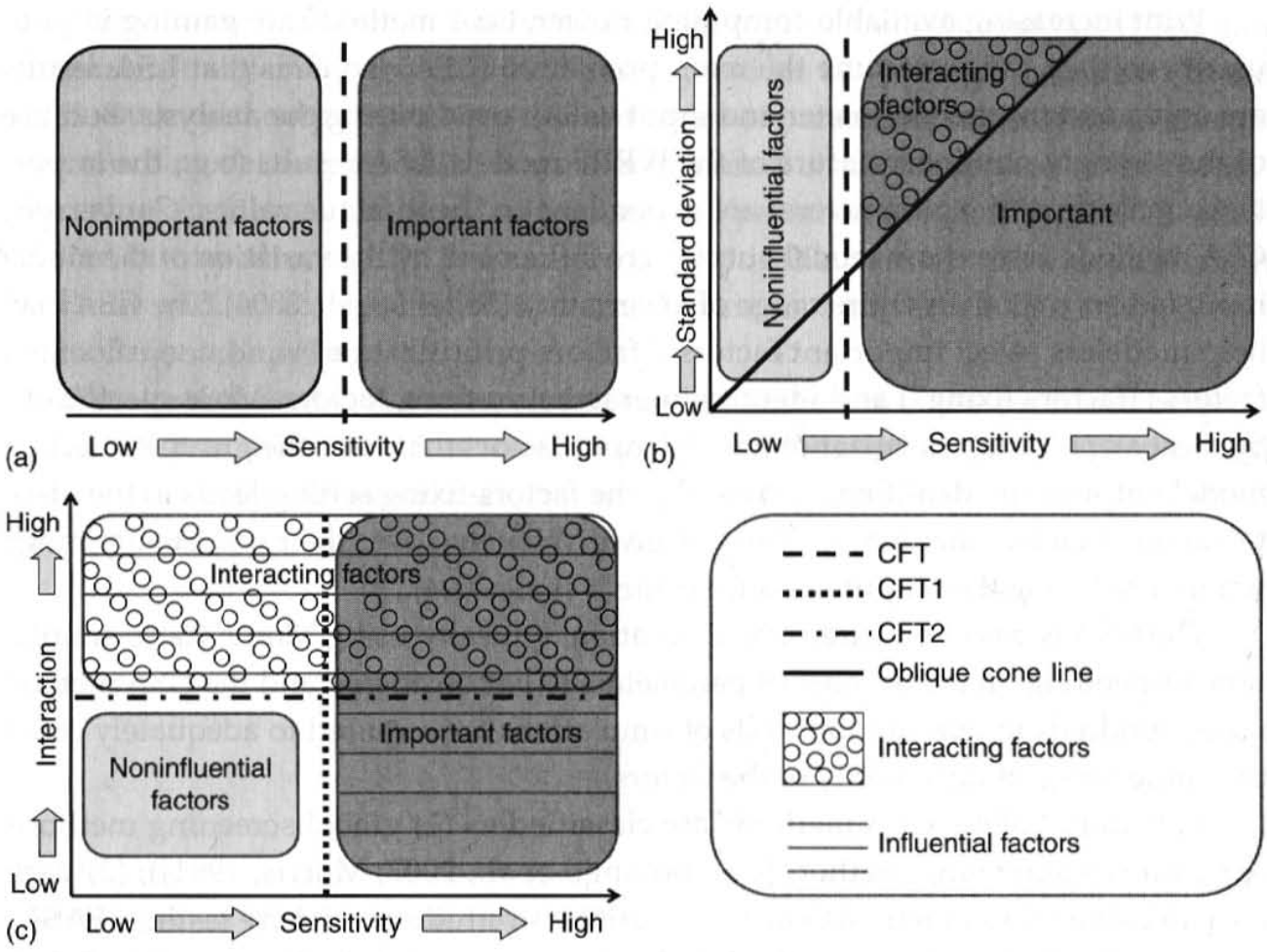

FIGURE 5.17 Schematic overview of the suggested terminology for differentiating input factors according to different GSA methods—(a) SRC, (b) Morris screening, and (c) E-FAST. (Mannina et al., 2012).

models (e.g., WRRF models), however, some nonimportant factors cannot be fixed because of interactions with other input factors (as discussed later in this section).

Morris screening provides a second type of classification of input factors. It allows for implicitly distinguishing between three different types of factors with respect to the mean and the standard deviation of the sensitivity, as follows (Figure 5.17b):

- Important factors—if mean sensitivity > CFT
- Interacting factors—if mean sensitivity > CFT and the standard deviation of the sensitivity is above a specified cone line
- Noninfluential factors—if mean sensitivity < CFT

In particular, the method as modified by Campolongo et al. (2007) basically defines a cone whose edges are set by a CFT and an oblique line that is a statistical function of the mean and standard deviation of the sensitivity (Figure 5.17b) (quantitative characteristics are given here).

The E-FAST method distinguishes four classes of factors on the basis of two CFTs (CFT1 and CFT2) as follows (Figure 5.17c):

- Important factors—if sensitivity > CFT1
- Interacting factors—if interaction > CFT2
- Influential factors—if sensitivity > CFT1 or interaction > CFT2
- Noninfluential factors—if sensitivity < CFT1 and interaction < CFT2

Noninfluential factors that can be identified by both Morris screening and the E-FAST method can be fixed anywhere within their range of uncertainty without changing the model output variance.

In terms of computational load, there is nonconclusive evidence that the SRC method is the least computationally expensive, followed by the Morris screening method and, finally, the E-FAST and Sobol methods. However, issues with convergence of the methods need to be studied further (Benedetti et al., 2011; Yang, 2011)

7.4 Uncertainty Analysis

In the field of wastewater treatment modeling, uncertainty analysis is increasingly recognized as an essential tool that, next to simulation results, also provides a quantitative expression of the reliability of those results (Belia et al., 2009). Next to the expression of uncertainty bounds on results, uncertainty studies can also be used to provide insight to the role of parameter and input uncertainty on model output uncertainty. Finally, uncertainty analysis can also be a means to prioritize dealing with uncertainties and to focus research efforts on the most problematic points of a model. As such, it helps to prepare future measurement campaigns.

The following steps can be taken to conduct a simple uncertainty analysis: (1) identification of the main uncertainty sources, (2) characterization of parameter and input uncertainty, and (3) propagation of the uncertainties into the model outputs.

7.4.1 Step 1—Identification of the Main Uncertainty Sources

In literature, sources of uncertainty have been considered from the perspective of where they are located in a generic model (Refsgaard et al., 2007; Walker et al., 2003). Thus,

these authors identified three or four main areas that introduce uncertainties to model predictions. These are model inputs (i.e., any type of data needed to perform a simulation; e.g., influent flow and wastewater characteristics); model structure (e.g., activated sludge model and clarifier model); and model parameters. Uncertainty in the inputs is caused by random variations of the system (e.g., weather) and to errors in measurements (e.g., imprecise sampling and measurement techniques). Uncertainty in the model is caused by incomplete understanding of the modeled processes and/or the simplified descriptions of the processes chosen to be included in models. A fourth source of uncertainty results from implementation of the models in software packages (e.g., numerical integration, bugs, and solver settings) (Claeys et al., 2010; Copp et al., 2008).

To provide a more intuitive method of identifying sources of uncertainty, Belia et al. (2009) proposed that the focus be shifted from the location of uncertainty within the model to when this uncertainty is introduced during a typical modeling project. To aid in this analysis, typical steps of a standard modeling project can be used (Refsgaard et al., 2005). The five steps, shown in the first row of Figure 5.18, are an intuitive sequence of tasks as suggested by the IWA Task Group on Good Modeling Practice (Rieger et al., 2012).

Uncertainty can be identified and evaluated at key times during a project as suggested by Refsgaard et al. (2007) and shown in Figure 5.18. This figure also includes a list of items for each project step that need to be selected or decided on and that identify a location of uncertainty. The figure, therefore, combines the traditional location of uncertainty within the model with a project-step-oriented or sequential approach.

Belia et al. (2009) provide an extensive list of the sources of uncertainty introduced during a typical modeling project.

7.4.2 *Step 2—Estimation or Calculation of Uncertainty*

Parameter uncertainty can be calculated from the covariance matrix. The latter is obtained during local sensitivity analysis or the calibration process if optimization methods are derivative-based so that the covariance matrix is calculated during optimization (Beck, 1987).

If no direct calculations are possible (e.g., for uncertainty on inputs, the uncertainties need to be estimated), one can divide the parameters and data in uncertainty classes (i.e., accurately known, very poorly known, and an intermediate class) and assign a percentage uncertainty to them. Reichert and Vanrolleghem (2001) adopted a similar approach to this. If direct calculation is impossible, other options are expert knowledge, questionnaires, or statistical calculation of uncertainties with historic data.

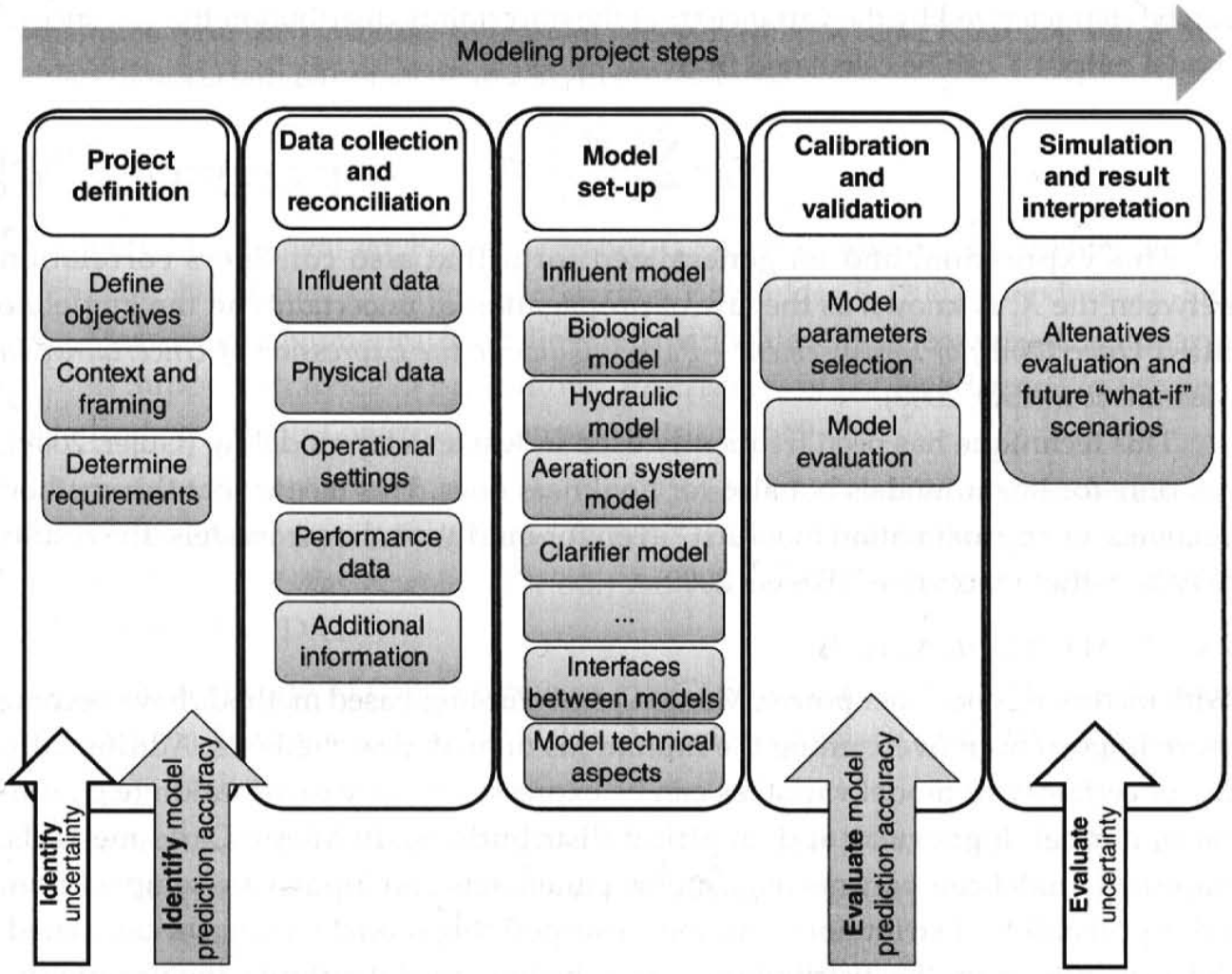

FIGURE 5.18 Typical modeling project steps including instances where model uncertainty and prediction accuracy should be identified and evaluated. (Adapted from Refsgaard et al. [2007] and Rieger et al. [2012]).

7.4.3 *Step 3—Propagate Uncertainty through the Model*

To propagate uncertainty in model outputs, different approaches are available that can be divided into the following two main groups: (analytical) uncertainty propagation equations or (probabilistic) Monte Carlo sampling-based methods.

7.4.3.1 *Error Propagation Equations*

Uncertainty can be propagated analytically through simple, linear, or nearly linear models. In the simple form of uncertain parameters and inputs X whose uncertainty

can be characterized by the variance σ_x^2 of the uncertainty distribution, the variance of model output Y can be calculated from

$$\sigma_y^2 = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 \cdot \sigma_i^2 \tag{5.18}$$

This expression, and its generalized form that also considers correlation between the X, is known as the law of propagation of uncertainty in the guideline titled *Uncertainty of Measurement—Part 3: Guide to the Expression of Uncertainty in Measurement* (ISO, 2008).

This technique has been frequently used in wastewater modeling (Gujer, 2009), not only for linear models but also for nonlinear ones. This means that this method becomes an approximation in which "even for mildly nonlinear models, the results may be rather inaccurate" (Beven, 2009).

7.4.3.2 Monte Carlo Methods

With increasing computer power, Monte Carlo sampling-based methods have become more important in overcoming the limitations of analytical methods. Additionally, the uncertainty of model variables can be expressed by any distribution (e.g., uniform, normal, lognormal, and empirical distributions). In Monte Carlo methods, uncertain model components (e.g., model parameters and inputs) are sampled from prior probability distributions and the corresponding model results are calculated. Subsequently, from the distribution of the obtained model outputs, the uncertainty bounds (e.g., 5% and 95% percentiles) can be calculated.

Different methods for sampling the parameter space that are used range from random (brute-force) sampling to optimized Monte Carlo methods as Markov Chain Monte Carlo simulations (Kuczera and Parent, 1998). In addition, structured sampling of the parameter space is possible through use of a variety of methods (e.g., Latin Hypercube sampling).

Despite significant progress in computational power during the last few years, the problem still persists that when dealing with a large number of parameters and inputs it is difficult to draw enough samples for an adequate representation of the models' output uncertainty distribution, especially when computational requirements and model run times are high. Benedetti et al. (2011) reviewed the number of simulations that are typically required to obtain an adequate representation and concluded that the number depends on the model used and even the output considered.

Overall, the necessary number of simulations varied between 15 and 150 times the number of uncertain parameters and inputs considered.

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Preface

Over the past 20 years, mathematical modeling of wastewater treatment processes has become the default tool for process design in many engineering firms throughout the world and is beginning to be used at operating facilities to help make day-to-day operating decisions. Increased computer processing power and user-friendly simulation software make it possible to model many of the complexities of a water resource recovery facility (WRRF) using personal computers. These simulators can be used to develop mass-balance models of the plant, linking several unit processes together and modeling their interactions. In addition, they can be used to carry out dynamic simulations to investigate diurnal and other transient behavior of a WRRF, such as the effect of wet weather.

With an increased use of process models through user-friendly simulators, there has been widespread acknowledgment in the industry that good training and expert guidance is needed to ensure that these models are developed, used, and documented correctly. This manual provides a broad range of information to help process engineers, operators, regulators, and owners understand general modeling concepts, terminology unique to computer modeling, and practical guidance and ideas on how to use process models for design and operation of small, medium, and large WRRFs. The modeling approach presented in this manual is consistent with the unified protocol proposed by the International Water Association task group on good modeling practice.

This publication was produced under the direction of Andrew R. Shaw, P.E., *Chair,* and Bruce R. Johnson, P.E., BCEE, *Vice-Chair.*

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Environmental Engineering

The Most Complete, Up-to-Date Guide to Process Modeling Methods and Protocols

Fully revised to cover the latest advances in the field, *Wastewater Treatment Process Modeling,* Second Edition, explains general modeling concepts and terminology and offers practical details on how to use process models for the design and operation of small, medium, and large water resource recovery facilities. This Water Environment Federation manual describes each step of the modeling process, including the fundamental math required, overviews of existing models and when to use them, modeling protocols, and how to interpret data. The detailed information in this authoritative volume helps to ensure that process models are developed, used, and documented correctly.

Coverage includes:

- History of process modeling
- Modeling fundamentals
- Unit process model descriptions
- Process modeling tools
- Dedicated experiments and tools
- Overview of available modeling and simulation protocols
- Project definition
- Building a facility model
- Using models for design, optimization, and control

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