

A framework for good biofilm reactor modeling practice (GBRMP)

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ABSTRACT

A researcher or practitioner can employ a biofilm model to gain insight into what controls the performance of a biofilm process and for optimizing its performance. While a wide range of biofilm-modeling platforms is available, a good strategy is to choose the simplest model that includes sufficient components and processes to address the modeling goal. In most cases, a one-dimensional biofilm model provides the best balance, and good choices can range from hand-calculation analytical solutions, simple spreadsheets, and numerical-method platforms. What is missing today is clear guidance on how to apply a biofilm model to obtain accurate and meaningful results. Here, we present a five-step framework for good biofilm reactor modeling practice (GBRMP). The first four steps are (1) obtain information on the biofilm reactor system, (2) characterize the influent, (3) choose the plant and biofilm model, and (4) define the conversion processes. Each step demands that the model user understands the important components and processes in the system, one of the main benefits of doing biofilm modeling. The fifth step is to calibrate and validate the model: System-specific model parameters are adjusted within reasonable ranges so that model outputs match actual system performance. Calibration is not a simple 'by the numbers' process, and it requires that the modeler follows a logical hierarchy of steps. Calibration requires that the adjusted parameters remain within realistic ranges and that the calibration process be carried out in an iterative manner. Once each of steps 1 through 5 is completed satisfactorily, the calibrated model can be used for its intended purpose, such as optimizing performance, trouble-shooting poor performance, or gaining deeper understanding of what controls process performance.

Key words | biofilm, framework, good practice, modeling, reactor

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NOTATION

Symbol/ abbreviation	Definition	Dimensions ^a
A_F	Biofilm surface area	L^2
BAF	Biological aerated filter	
D	Substrate diffusion coefficient in the bulk liquid	$L^2 T^{-1}$
D_F	Substrate diffusion coefficient in the biofilm	$L^2 T^{-1}$
DO	Dissolved oxygen	$M L^{-3}$
IFAS	Integrated fixed-film activated sludge	
J_F	Substrate flux into the biofilm from the bulk liquid	$M L^{-2} T^{-1}$
K	Half-maximum-rate concentration	$M L^{-3}$
k_{attach}	Rate coefficient for attachment from the bulk to the biofilm	Variable ^b
k_{detach}	Rate coefficient for detachment from the biofilm to the bulk	Variable ^b
$k_{L,a}$	Gas-liquid transfer coefficient	T^{-1}
L_F	Biofilm thickness	L
$(L_{L,i})$	Mass transfer boundary layer thickness (index i : different L_L in different stages of the reactor system)	L
MBBR	Moving-bed biofilm reactor	
MBfR	Membrane biofilm reactor	
\hat{q}	Maximum specific rate of substrate utilization	$M_{substrate} M_{biomass}^{-1} T^{-1}$
RBC	Rotating biological contactor	
S	Substrate concentration in the bulk liquid where substrate is a generic term that can relate to any of the rate-limiting compounds such as organic substrate, NH_4^+ , NO_3^- , or O_2	$M_{substrate} L^{-3}$
S_B	Soluble (readily) biodegradable organic substrate	$M_{substrate} L^{-3}$
S_F	Substrate concentration inside the biofilm	$M_{substrate} L^{-3}$
$S_{L,F}$	Substrate concentration at the outer surface of the biofilm	$M_{substrate} L^{-3}$
SOTE	Standard oxygen transfer efficiency	–
TSS	Total suspended solids	$M_{solids} L^{-3}$
UASB	Upflow anaerobic sludge blanket	
VSS	Volatile suspended solids	$M_{solids} L^{-3}$
X_F	State variable that quantifies particulate components in a biofilm (biomass per unit biofilm volume). Most biofilm models and simulators consider different types such as heterotrophic biomass ($X_{OHO,F}$), autotrophic nitrifying biomass ($X_{ANO,F}$), and unbiodegradable particulate biomass ($X_{U,F}$). The sum of these particulate components corresponds to the overall measured $X_{Tot,F}$. Note that the value of the different X_F may be constant (as is assumed in Equation (1)) or may vary over the biofilm thickness (Wanner <i>et al.</i> 2006)	$M_{solids} L^{-3}{}^c$
$X_{Tot,A}$	Amount of biomass in the biofilm per unit substratum area (Note: $X_{Tot,A} = X_{Tot,F} L_F$)	$M_{solids} L^{-2}$
$X_{Tot,F}$	Concentration of biomass in the biofilm (biomass per unit biofilm volume) where biomass is typically quantified as VSS, TSS, or COD. In other references $X_{Tot,F}$ is sometimes referred to as biofilm biomass density of biofilm biomass concentration (Note: $X_{Tot,F} = X_{Tot,A}/L_F$)	$M_{solids} L^{-3}{}^c$
X_U	Particulate unbiodegradable organic matter concentration	$M_{solids} L^{-3}$
z	Distance dimension perpendicular to the biofilm surface	L
α	Ratio of the wastewater to clean water oxygen mass transfer coefficient	–

^aDimensions are defined according to the SI base quantities L for length, M for mass, T for time. Nomenclature is based on Wanner *et al.* (2006) and Corominas *et al.* (2010).

^bDepends on the type of rate expressions used (e.g., Table 17.4 in Morgenroth 2008).

^cConcentrations in the biofilm are per unit volume biofilm and not per overall reactor volume. For simple (planar) biofilm geometries the definition of the biofilm volume is straightforward. For heterogeneous structures the unit biofilm volume considers only the space occupied by particulate components and not the pore space. See also corresponding discussion related to Figure 2.2(c) in Wanner *et al.* (2006).

INTRODUCTION

It would not be an exaggeration to say that the development and adoption of the International Water Association (IWA) activated sludge models (ASMs), along with their incorporation into plant-wide modeling protocols, has transformed wastewater-treatment education, research, and practice (Daigger 2011). Since their introduction (Henze *et al.* 1987), these models have become the accepted means of evaluating, designing, and assisting with the operation of water resources recovery facilities (WRRFs) using the activated sludge process in its many variations. This is because the models and associated protocols meet the criteria for useful application. First, they are based on a combination of sound science and engineering, and are scalable to provide the level of detail necessary to address real-world challenges. Second, the models have kept the complexity as low as possible while encompassing truly important components and processes. Third, a strong experience base has accumulated to allow their reliable application. Finally, their widespread application provides a common understanding and language that facilitate communication between researchers and practitioners, beginning with the instruction of students learning about biological water resources recovery.

Why do we use models of biological processes? First and foremost, models are efficient ways of incorporating known and relevant science, engineering, and practice into an executable tool. On the one hand, the results of their proper application can be relied upon for their generalizable accuracy, in comparison to empirical design criteria, which are site and situation specific. On the other hand, model failures in specific applications identify areas needing further research. In this way, the routine and consistent application of accepted models drives the improvement of fundamental understanding and practice.

Models with firm mechanistic and experiential bases can be used reliably to establish design and operating criteria for WRRFs, resulting in more efficient and effective operation. They also can be used for troubleshooting, *i.e.*, identifying the reasons for operating difficulties and necessary corrective actions. Likewise, models can be used to determine the operating limits for existing facilities, along with methods to optimize and further increase capacity and performance.

While the ASMs provide these kinds of tools for WRRFs based on suspended-growth processes, biofilm-based processes do not have analogous well-established linkages to biofilm models. This deficiency cannot be fixed by applying

ASMs to biofilm processes, because of the profound importance of mass-transport processes in biofilms, along with process kinetics (Boltz & Daigger 2010).

While a plethora of biofilm models exist (Wanner *et al.* 2006), no consistent and widely used protocol is available to guide the use of biofilm models to design and operate biofilm reactors. This lack of agreed-upon methodology for using biofilm models has been a barrier to the implementation of biofilm reactors in WRRFs.

What if an agreed-upon means to use biofilm models were in place? Examples of the practical questions that could be addressed by a biofilm model include: (1) What is the achievable flux of ammonium nitrogen ($\text{NH}_4^+\text{-N}$), thereby allowing the required size of the biofilm reactor to achieve a specified effluent concentration to be determined? (2) Why is my biofilm reactor not performing as well as needed (*e.g.*, insufficient biochemical oxygen demand (BOD), removal or the production of nitrate nitrogen, $\text{NO}_2^-\text{-N}$)? (3) Why does process performance vary from summer to winter, and what can I do about it? (4) What is the biofilm carrier requirement and associated reactor size for the different types of biofilm reactors I am considering? (5) How do biofilm-carrier features affect important biofilm characteristics, such as surface area, detachment rate, and biomass accumulation? It is easy to see the practical value of a reliable and robust protocol for modeling biofilm reactors.

In this paper, we present a framework for good biofilm reactor modeling practice (GBRMP). We first provide a succinct overview of available biofilm models; we conclude that one-dimensional (1D) models generally are sufficient for engineering practice. We then outline a five-step GBRMP framework. It is structured along the lines of the widely used good modeling practices framework for activated sludge (Rieger *et al.* 2013), but with essential differences related to biofilm reactors.

Based on the GBRMP framework, we provide guidance for selecting the appropriate 1D biofilm model, and we follow up with simple examples of applying the framework. We conclude with a discussion of the need for model calibration and validation when modeling biofilm reactors.

AN OVERVIEW OF BIOFILM MODELS

Biofilm modeling began in the mid-1970s with the seminal works of Atkinson & Davies (1974), Williamson & McCarty (1976), and Harremoës (1976). The key to each of these early works was recognizing that the rate of mass transport of substrate into the biofilm could limit system performance as

much as the degradation potential by the bacteria inside the biofilm. Using straightforward 1D reaction and diffusion models, these early leaders showed how substrate concentrations decline with distance into the biofilm. The bacteria inside the biofilm often experience a much lower substrate concentration than those in the bulk liquid or at the outer surface of the biofilm.

Over four decades have passed since the work of the pioneers of biofilm modeling. Biofilm modeling has grown in scope, sophistication, and power. Wanner *et al.* (2006) published a comprehensive review of biofilm models, and the reader can find in it excellent details about the structure and use of biofilm models. Here, we provide a succinct overview of the key features of biofilm models.

Components and processes

A biofilm model is simply a set of mass-balance equations that are solved simultaneously. The core of a biofilm model involves defining the components and processes that are to be represented by the mass balances. The components are divided into two broad categories: the microorganisms and the materials that the microorganisms consume or produce. For modeling biofilms used in wastewater treatment, some important sets of components are as follows:

- Heterotrophic bacteria that consume biochemical oxygen demand (BOD) and dissolved oxygen (DO).
- Nitrifying bacteria that consume NH_4^+ and DO, and produce NO_3^- .
- Denitrifying bacteria that consume NO_3^- and BOD.

For the three sets of components, the microbiological processes are, respectively, aerobic oxidation of BOD, nitrification of NH_4^+ , and denitrification of NO_3^- .

If we want to model all three processes, we need at least seven mass balances: aerobic heterotrophs, nitrifying bacteria, denitrifying bacteria, BOD, DO, NH_4^+ , and NO_3^- . The first three components are solids that form the biofilm. The last four components are soluble materials that can move through the biofilm. If we are only interested in aerobic removal of BOD, the mass balance can be simplified to aerobic heterotrophs, BOD, and DO. If DO is not limiting, then the mass balances can be simplified further to heterotrophs and BOD.

While this seven-component, three-process scenario is widely applicable, it is only one simple example of systems that can be represented by biofilm models. Other components and processes that can be incorporated into biofilm models include inert biomass, extracellular polymeric

substances (EPS), refractory organic compounds, anaerobic ammonium oxidation (anammox) bacteria, sulfur-reducing and -oxidizing bacteria, and organic micro-pollutants.

In addition to microbiological processes, we must include mass-transport processes, because the substrates need to move from the bulk liquid to the microorganisms inside the biofilm. The mass-transport processes include diffusion or something that can be described by analogy to diffusion. They are driven by a concentration gradient, which explains why concentration gradients must develop in biofilms. Without a concentration gradient, the substrates cannot get to the bacteria inside the biofilm. Mass transport is important inside the biofilm and also for moving the substrates from the bulk liquid to the outside of the biofilm. The latter is called external mass transfer; it is controlled by the turbulence in the water moving past the biofilm, and the result is a concentration gradient between the bulk liquid and the outer surface of the biofilm.

Equations (1) and (2) give a simple example of steady-state mass balances for a single substrate inside a 1D biofilm. Equation (1) shows the balance of diffusion and microbial utilization inside the biofilm. Equation (2) shows how external mass transfer provides the same flux of substrate from the bulk liquid as into the biofilm.

$$0 = D_F \frac{d^2 S_F}{dz^2} - \frac{\hat{q} X_F S_F}{K + S_F} \quad (1)$$

$$J_F = \frac{D}{L_L} (S - S_{LF}) = D_F \frac{dS_F}{dz} \Big|_{z=0} \quad (2)$$

S = substrate concentration in the bulk liquid, S_{LF} = substrate concentration at the outer surface of the biofilm, S_F = substrate concentration inside the biofilm, \hat{q} = the maximum specific rate of substrate utilization, K = the half-maximum-rate concentration, X_F = concentration of active biomass in the biofilm, D_F = substrate diffusion coefficient in the biofilm, D = substrate diffusion coefficient in the bulk liquid, J_F = the substrate flux from the bulk liquid into the biofilm, L_L = the mass transfer boundary layer thickness, and z = the distance dimension perpendicular to the biofilm surface. A detailed discussion of assumptions, boundary conditions, and solutions of Equations (1) and (2) is provided in the report by Wanner *et al.* (2006) or in related textbooks (Rittmann & McCarty 2001; Morgenroth 2008).

Other important transport processes are the detachment of biomass from the biofilm and the attachment of suspended solids onto the biofilm. Detachment can be represented in several ways (Wanner *et al.* 2006), and it

affects the total amount of metabolically active biomass that accumulates. If the detachment rate is slower than the net rate of biomass synthesis, the active biomass accumulates, or grows. A faster detachment rate causes the active biomass to shrink. Attachment of suspended solids also affects the total amount of biofilm and how much of it is active biomass versus non-active solids.

Multi-dimensional models

A very important feature of modern biofilm modeling is that the biofilm can also be represented in two or three dimensions, i.e., as 2D and 3D models (Wanner *et al.* 2006). Modeling more than one dimension makes it possible to represent complex changes in the physical morphology of biofilms, as well as hydrodynamic interactions between the biofilm and the water flowing past the biofilm. Multi-dimensional models also allow more sophisticated treatment of complex ecological interactions that occur inside some biofilms. All of these features can be accentuated by recent developments using continuum as well as cellular-automaton and individual-biomass models, along with movie-style visualization of the outputs.

While multi-dimensional models add a great deal of power to biofilm modeling and can offer exceptional insights into phenomena that occur in some settings, they demand heavy computing resources and deep programming expertise. Thus, 2D and 3D models are used today as research tools, but are not realistic for use by engineers to solve practical problems. Fortunately, a good 1D model can address all of the important questions that engineers need to address. This is true because the dominant processes in all biofilm settings are microbiological reaction and mass transport, which are captured well by a 1D model.

One-dimensional models

Wanner *et al.* 2006 give a comprehensive description of the types of 1D models available today. In brief, 1D models can be broken into three major types. *Analytical models* make simplifying assumptions so that Equation (1) can be solved with a closed-form analytical equation (Harremoes 1976; Rittmann & McCarty 2001). Examples of simplifying assumptions are using first-order or zero-order kinetics for the microbiological reaction and neglecting external mass-transfer resistance by assuming that $S = S_{LF}$. *Pseudo-analytical models* involve algebraic approximations to the numerical solutions to Equations (1) and (2) (and sometimes also a mass balance on the biomass) (Rittmann & McCarty

2001; Morgenroth 2008). They avoid the assumptions of analytical solutions and can be implemented with a simple spreadsheet for a limited number of components and processes (Wanner *et al.* 2006). *Numerical models* use computer techniques to solve the set of mass-balance equations. A convenient and often-used tool is AQUASIM (Wanner & Morgenroth 2004; Wanner *et al.* 2006). Numerical solutions require the fewest simplifying assumptions and can be used to solve systems with many components and processes.

Although the following discussion of the GBRMP framework focuses on using 1D numerical models, it is appropriate for any type of biofilm model.

SELECTING A 1D MODEL

With limited understanding of biofilm processes, a novice modeler may be tempted to 'play it safe' by choosing the most complex biofilm model available. While this strategy might work out well for activated sludge modeling (Grau *et al.* 2009), it is not advisable for biofilm reactor modeling. One reason is that computing time often is a limiting factor for biofilm reactor modeling, and excess complexity increases the computational time by orders of magnitude. A second reason is that a complex biofilm model will require that the user provides many input parameters that are difficult to determine and for which no reliable default parameters have been defined. Choosing a too-complex model will incur many penalties for producing output that does not improve the usefulness for the user.

The following examples provide guidance for deciding on a suitable model complexity. Figure 1 provides schematics of different modeling levels that correspond to the examples.

Flux of the limiting substrate

As an example, we consider the use of mathematical modeling to guide the design of a nitrifying moving-bed biofilm reactor (MBBR). The reactor can be assumed to be completely mixed, and the target effluent ammonium concentrations are low. Based on some simple calculations (e.g., Morgenroth 2008) the engineer has determined that the biofilm will be limited by NH_4^+ and not by DO. Because this system is limited by a single substrate, a range of analytical, pseudo-analytical, and numerical biofilm models can be applied to calculate the NH_4^+ flux and, from that, the necessary surface area of biofilm carrier. If

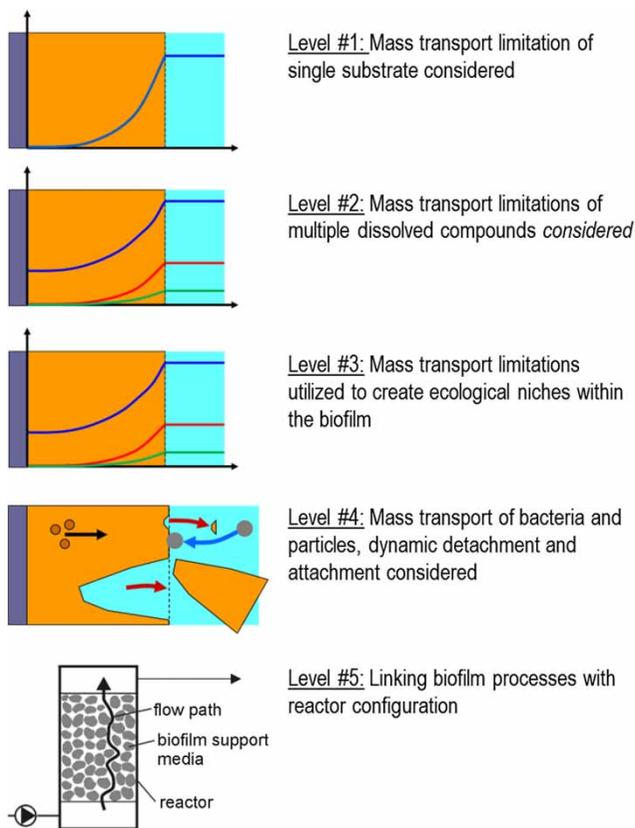


Figure 1 | Five levels of increasingly complex biofilm models (Levels 1–4) and integrating modeling results in the overall system design (Level 5). Note that level of complexity for the modeling of Levels #2 and #3 is identical; the difference is in the process objectives that in Level #3 consider the benefits resulting from mass-transport limitations (e.g., different redox zones within the biofilm).

the design also requires the DO flux, it can be estimated from the NH_4^+ flux based on the known stoichiometry of NH_4^+ and O_2 utilizations in nitrification (Level #1 in Figure 1).

Flux of the non-limiting substrate

To design a nitrifying biofilter, the engineer needs to estimate NH_4^+ and DO fluxes into the biofilm along the length of the reactor. Due to the relatively high influent NH_4^+ concentration, it can be assumed that, in the front part of the biofilter, the reaction is DO-limited, whereas NH_4^+ is rate limiting towards the outlet of the filter. A 1D numerical model that takes into account dual substrate limitations would be appropriate. In addition, the model needs to take into account changes in the bulk phase concentrations along the length of the biofilter, such as by modeling several biofilm compartments in series (Level #2 in Figure 1).

Competition for substrate and space

A biofilm reactor must oxidize dissolved organic carbon and NH_4^+ . Three soluble components need to be considered: organic substrate (represented as BOD or chemical oxygen demand (COD)), NH_4^+ , and their common electron acceptor, DO. Two unique groups of bacteria must be represented: faster-growing heterotrophic bacteria oxidizing the organic substrate and slower-growing autotrophic bacteria oxidizing NH_4^+ . Because performance depends on the relative penetration of the soluble substrates and also on the spatial distribution of the two groups of bacteria (Wanner & Gujer 1985), a mathematical model must explicitly represent the spatial distribution of all soluble substrates and biomass types. Many simulators, such as AQUASIM, allow this level of detail (Wanner & Morgenroth 2004; Boltz *et al.* 2010). Depending on the type of reactor, it may be suitable to assume a constant biofilm thickness or a constant detachment rate (Level #2 in Figure 1).

Beneficial use of partial penetration

The engineer wants to predict the performance of an aerobic biofilm reactor in which mass-transport limitations help to create unique local ecological niches: aerobic processes towards the outer surface and anoxic or anaerobic processes towards the core of the biofilm. A numerical model must be used to represent substrate transport and biomass distribution within the biofilm. The model needs to describe production and consumption of intermediates (e.g., NO_3^- and nitrite (NO_2^-)) and processes (e.g., denitrification) occurring inside the biofilm based on the intermediates. Thus, the biofilm must be sub-divided into sufficiently small numerical segments (or layers) to be able to represent different redox zones. Most commercial simulators allow for such representations (Level #3 in Figure 1).

Growth, detachment, and attachment

The engineer wants to model the fate of soluble and particulate organic carbon in an MBBR. While the approach for modeling soluble substrate is well established (e.g., Equations (1) and (2)), how to describe the fate of particles within a biofilm reactor is uncertain. Attachment, detachment, and transport of particles depends on the biofilm's physical structure. Mechanisms of particle attachment, detachment, and hydrolysis have to be represented, despite uncertainty. Many biofilm reactor simulators include

approaches to model particle attachment, but the lack of understanding of the actual mechanisms makes use of such built-in features risky. The modeler often must implement novel features based on the best understanding of the mechanisms affecting attachment and detachment (Level #4 in Figure 1).

Practical reactor implementation

In some cases the performance of a biofilm reactor is not determined as much by substrate flux as by physical phenomena, such as mixing, clogging of the carrier in a biofilter, and carrier distribution in an MBBR. Mathematical modeling can help understand possible biological causes of some of these problems (e.g., too much biofilm accumulation), but many problems are more related to details of mechanical equipment or complex fluid dynamics. Such features sometimes cannot be represented by commercial simulators used for biofilm reactor modeling. In this case, the modeler has to acknowledge that a 1D biofilm model will not be sufficient to solve the problem (Level #5 in Figure 1).

GBRMP FRAMEWORK

This section introduces a framework for the systematic step-by-step implementation and calibration of a mathematical model for a biofilm reactor (Figure 2). The framework was developed to describe biofilm reactors with suspended support media (e.g., the MBBR and integrated fixed-film activated sludge (IFAS)), but the underlying principles will be applicable to fixed-bed systems (e.g., biofilters and trickling filters) and to aerobic granular sludge systems. This framework is focused on basic principles, and it builds on experience from published reports on various aspects of biofilm reactor modeling: structured step-by-step approaches (Vigne *et al.* 2007; Vigne *et al.* 2010; Barry *et al.* 2012; Eldyasti *et al.* 2012); colloidal organic matter (Albizuri *et al.* 2009; Albizuri *et al.* 2014), laboratory-scale MBBRs (Vangsgaard *et al.* 2013), predation (Revilla *et al.* 2016), sensitivity and identifiability (Brockmann *et al.* 2008; Brockmann & Morgenroth 2010; Boltz *et al.* 2011; Brockmann *et al.* 2013), and experimental approaches to determine external mass transfer resistance (Nogueira *et al.* 2015).

Step 1: obtain information on the biofilm reactor system

Responsible application of a biofilm reactor model requires a good understanding of the actual biofilm reactor system to

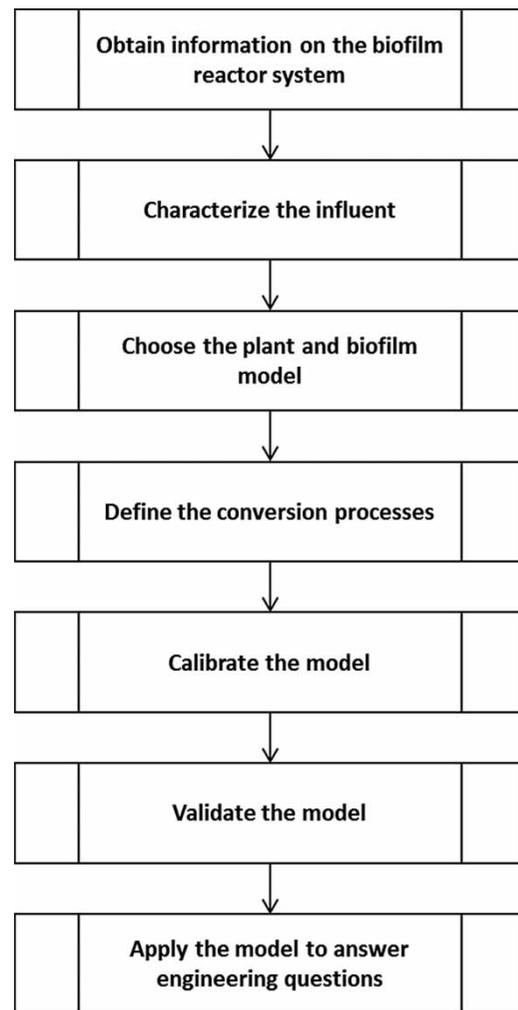


Figure 2 | Overall approach for good biofilm reactor modeling practice.

be evaluated. This system-level understanding includes knowing reactor volumes, mixing conditions (water and biofilm media), available biofilm surface area (A_F), microbial processes, oxygen transfer, and mechanisms and dynamics of detachment and biofilm thickness control (Table 1).

Step 2: characterize the influent

Wastewater flow and composition must be quantified in terms of average loadings, but also in terms of variability of flow and concentration of individual components (Table 1). In many cases, reactor performance will be impaired by varying loading. Biofilm reactors typically have a smaller hydraulic retention time (HRT) compared to activated sludge systems and, therefore, have less hydraulic buffering and higher sensitivity to hydraulic variations.

Table 1 | Recommended data requirements for GBRMP

Plant and operational information	Wastewater characteristics	Reactor and biofilm information
<ul style="list-style-type: none"> - Flow rates (influent and recycles) - Chemical dosing - Water distribution into reactors - Containment structure - Aeration devices and control - Mixing devices and control - Hydrodynamic mixing conditions - Carrier retention and water collection systems 	<ul style="list-style-type: none"> - Wastewater composition (total and filtered COD, readily biodegradable COD (S_B), $\text{NH}_4^+\text{-N}$, $\text{NO}_2^-\text{-N}$, $\text{NO}_3^-\text{-N}$, total Kjeldahl nitrogen (TKN) or total nitrogen, $\text{PO}_4^{3-}\text{-P}$, total P), VSS, TSS - Internal recycle flow composition - Daily and seasonal variability 	<ul style="list-style-type: none"> - Mixed liquor suspended solids (MLSS) and mixed liquor volatile suspended solids (MLVSS) of suspended biomass - Amount of biofilm per carrier surface ($=X_{\text{Tot,A}}$) - Biofilm surface area (A_F) - Biofilm thickness (L_F) and concentration of biomass in the biofilm ($X_{\text{Tot,F}}$) - P-content of biomass - Sludge volume index (SVI) of suspended biomass - Bulk liquid DO - Temperature - pH

In principle, wastewater composition can be characterized following procedures developed for activated sludge systems (Chapter 5.2 in Rieger *et al.* 2013). While the chemical composition (e.g., COD) is independent of whether the wastewater is treated in an activated sludge or a biofilm system, the size characterization should reflect retention and degradation mechanisms (Corominas *et al.* 2010). In biofilm systems, soluble compounds are transported into the biofilm by diffusion, and the corresponding diffusion coefficient must be quantified. Colloidal and particulate components of COD must be evaluated to determine to what extent they are transported into the biofilm, attach to the biofilm, or pass through the system. Thus, the terms soluble, colloidal, and particulate refer, on the one hand, to particle size, but also, on the other hand, to removal mechanisms. Therefore, retention may be different for activated sludge and biofilm systems.

Step 3: choose the plant and biofilm model

Flow and retention of water streams, suspended particles and biomass, and biofilm carriers with biofilm have to be characterized and implemented in the mathematical model. Note that a reactor may be plug flow for the water stream and suspended particles, but completely mixed for biofilm carriers with biofilm in a specific stage or within the overall biofilm system (Rittmann 1982; Boltz *et al.* 2017).

The biofilm itself is typically represented using a 1D layered model (Wanner *et al.* 2006). For many applications, three to 10 layers are sufficient. Most commercially available simulators set the default number of layers to values between three and 10; thus, the user must be alert to increase the number of layers if needed. For thick and heterogeneous biofilms, more layers may be needed, but increasing the number

of layers significantly increases computational time. The number of layers should be chosen based on an understanding of the biofilm thickness and the heterogeneity of process conditions within the biofilm. For example, if the aerobic zone towards the surface of the biofilm is in the order of 100 μm thick, the thickness of a single layer must be 100 μm or smaller. A rough rule of thumb is that the number of layers can be estimated by dividing the biofilm thickness by the thickness of the smallest process zone in the biofilm.

Biofilms are in many cases mass-transport limited, and model predictions are more sensitive to biofilm surface area and external mass transfer resistance than to the overall amount of biomass. In that case, the modeler must either fix a certain biofilm thickness (e.g., based on measurements in the full-scale reactor) or have the model predict biofilm thickness (e.g., by fixing the value of the detachment and attachment rate coefficients). Detachment has a particularly strong influence on biofilm thickness and also on ecological niches for slow-growing microorganisms within the biofilm (Rittmann & Manem 1992; Rittmann *et al.* 2002). Attachment of particulate and colloidal components also influences the availability of organic substrate within the biofilm and the seeding of the biofilm by suspended biomass. In addition to determining the average biofilm thickness, the modeler also must decide on considerations relating dynamic changes of biofilm thickness or biofilm detachment and decide on rate expressions for particle hydrolysis (Janning *et al.* 1998; Morgenroth *et al.* 2002; Hauduc *et al.* 2013). Biofilm detachment, attachment, and corresponding biofilm thickness (average or dynamically varying) can under some conditions have a significant influence on biofilm reactor performance, but are to-date still not well understood (Morgenroth & Wilderer 2000; Morgenroth 2003). It is the responsibility of the model user to understand

the implications of uncertainty in biofilm thickness or detachment modeling.

Step 4: define the conversion processes

Conversion processes in biofilm reactors – such as BOD and NH_4^+ oxidation or denitrification – are similar to processes in activated sludge. Therefore, the existing mathematical process models developed for activated sludge systems (Henze 2000) can be adapted for biofilm reactors. A key difference between activated sludge and biofilm models is that biofilm models take mass transfer resistances explicitly into account, while, for activated sludge systems, the effect of mass transfer resistance into the floc typically is implicitly modeled by choosing a larger value of the half-maximum-rate concentrations (K). Thus, in biofilm reactor models, the value of the half-maximum-rate concentrations often is significantly smaller (e.g., 10% of the value in the activated sludge model) compared to default values in Henze (2000). When modeling IFAS systems, it will be necessary to use different values for half-maximum-rate concentrations for suspended biomass and for biomass in biofilms.

Different processes may be limiting in biofilm reactors compared to activated sludge processes. For example, biofilm reactors more commonly experience NO_2^- accumulation compared to activated sludge systems; hence, it may be more important to implement a two-step nitrification model when modeling biofilm processes, even if one-step nitrification works well for activated sludge.

Step 5: calibrate/validate the model

Model calibration adjusts system-specific model parameters within reasonable ranges so that relevant model predictions match actual system performance. Ideally, a first comparison should be done for steady-state operation and model predictions. This is more likely in laboratory and pilot plants, where influent conditions and reactor operation can be kept constant for sufficiently long to approach steady state. Practical biofilm reactors almost always will have variability in the influent and often also in reactor operation. Achieving steady state in a biofilm simulation can be quite time consuming due to the many interactions among components and processes. A common mistake, used to save time, is to start with some random initial conditions and simply simulate for a few days. This mistake should be avoided, and simulations should be run until all components reach stable outputs. It can require several months of simulated time to reach steady state.

Because biofilm models are complex, model predictions often are non-linearly related to model input parameters. Furthermore, many of the model's output values are correlated for a range of modeling scenarios. While some model parameters (e.g., biofilm thickness) may have no influence on model predictions in certain situations (e.g., for thick biofilms and for low bulk phase substrate concentrations resulting in deep biofilms), the same parameter may have a dominant influence on model predictions in other settings (e.g. a thin biofilm with rapid external mass transfer). Thus, parameter sensitivities are linked to initial values chosen (Brockmann *et al.* 2008). Regardless of this complexity, it is still possible to obtain relevant model predictions by following a structured approach and by taking into account parameter uncertainty when interpreting modeling results.

The calibration process should follow a hierarchy by which the most situation-specific parameters are adjusted first, while the most well-established parameters are maintained. For example, if the model is not producing results that correspond to the actual performance, the strategy for adjusting parameters should follow this sequence. First, the physical parameters – e.g., flow rates, volumes, and surface areas – should be double-checked. If that fails to fix the problem, the second step is to re-evaluate the influent characteristics. Third is to adjust biofilm parameters, such as biomass accumulation and external mass-transfer boundary layer thickness. Only if all of the preceding adjustments fail should the user resort to adjusting kinetic and, lastly, stoichiometric values.

Model calibration usually works best when performed sequentially following four steps: (1) biomass on carriers, (2) COD or BOD removal, (3) nitrogen removal, and (4) aeration. Figure 3 lays out a stepwise procedure for calibration. The following sub-sections describe typical procedures for each step of calibration.

Calibrating biomass on carriers

Determine a realistic biofilm surface area for each reactor stage, and quantify the amount of biofilm biomass in the different reactor stages (calibration step 1a)

In most cases, the supplier of the biofilm support media can provide the specific surface area for the medium (in m^2 biofilm surface per m^3 of reactor volume or per m^3 of added media volume). Note that this specific surface area can depend on reactor operation; under certain conditions, the actual value is actually larger than reported by the manufacturer (e.g., due to the formation of streamers on the biofilm that increase the available surface area) or smaller than

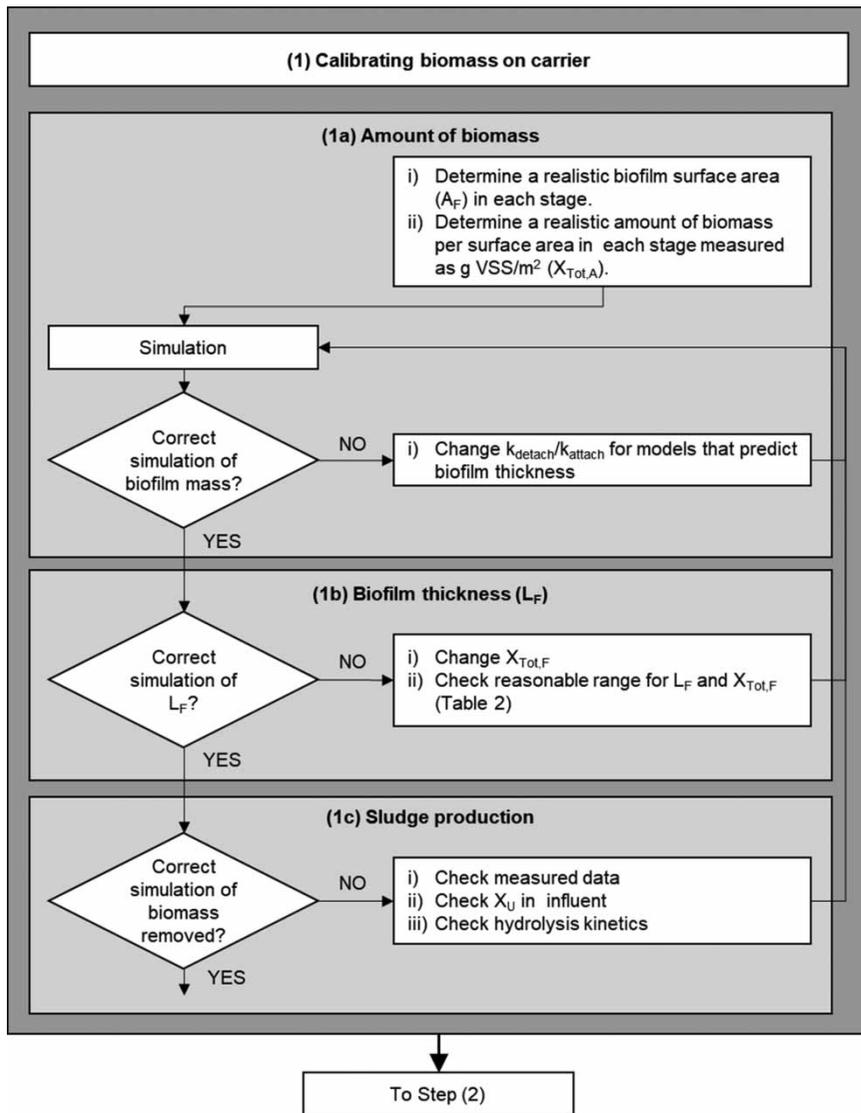


Figure 3 | Stepwise calibration of a biofilm reactor model. Calibration should follow this general sequence, but ultimately may need additional cycling through the calibration steps. (Continued.)

reported by the manufacturer (e.g., if pores or a heterogeneous surface of the support media are fully overgrown by biofilm). The actual available specific surface area may change with influent substrate loading, between winter and summer, from startup to long-term operation, due to predation, or due to changes in mechanical forces (e.g., through changes in the fill ratio or aeration intensity).

For an operating biofilm plant, the amount of biofilm biomass can be measured by sampling a known amount of media from different stages and measuring VSS. Based on the VSS per removed carrier and the specific surface area of the carrier, the amount of biomass per surface area (A_F) can be calculated. The measured amount of biomass

should then be compared to model predictions. The model can be calibrated to match the observed biomass by adjusting detachment and/or attachment coefficients (if the biofilm thickness is predicted by the model) or by adjusting the biofilm thickness (L_F) or the concentration of biomass in the biofilm ($X_{Tot,F}$) (if the biofilm thickness is fixed; see also next step).

Biofilm thickness (calibration step 1b)

Once the biomass per surface area ($= X_{Tot,A} = X_{Tot,F} \cdot L_F$) is fixed, then the combination of biofilm thickness (L_F) and biomass concentration ($X_{Tot,F}$) must be chosen to match

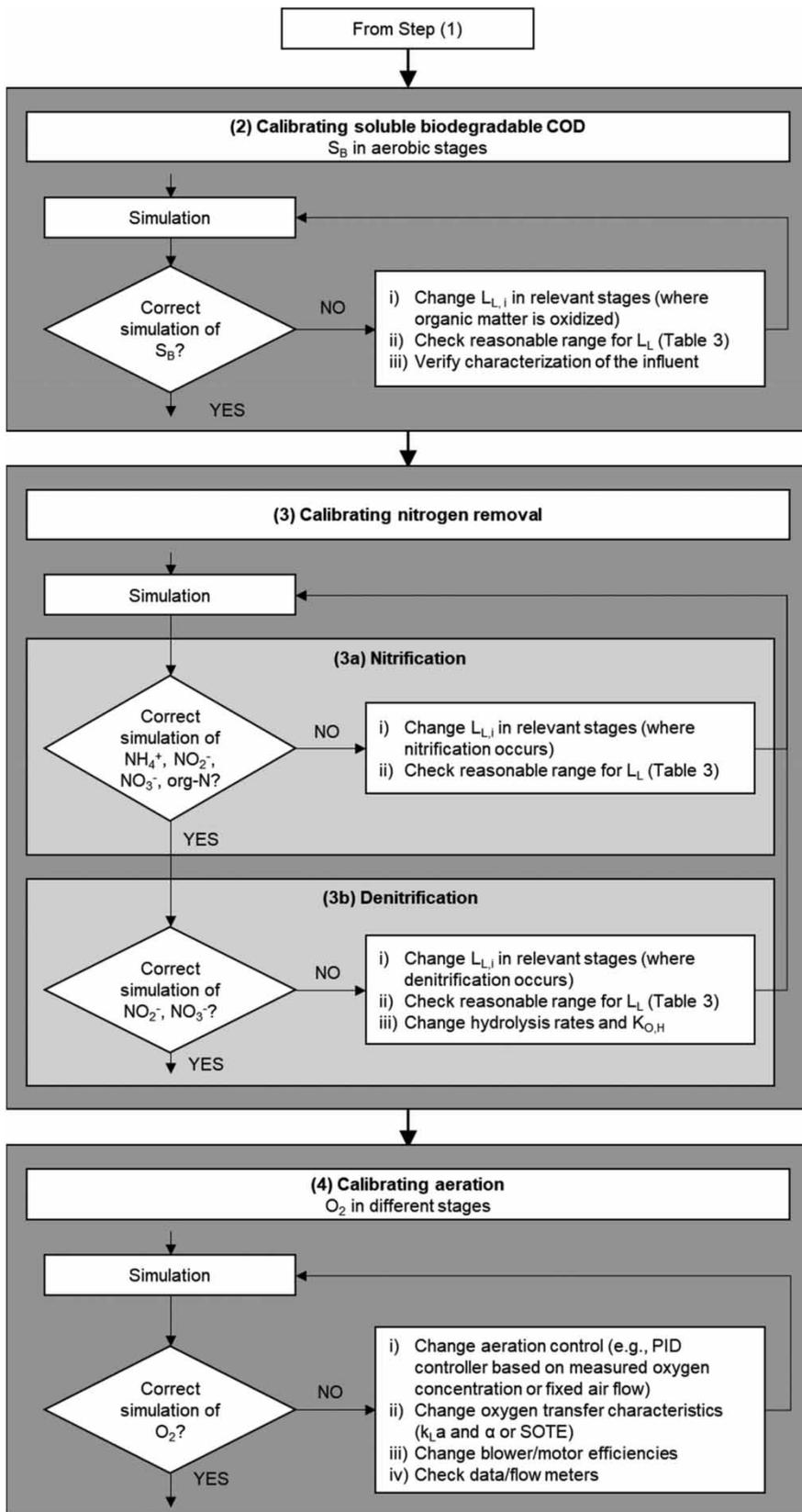


Figure 3 | Continued.

this value. Ideally the biofilm thickness should be measured for the actual biofilm reactor (e.g., microscopically after sampling a number of carriers, e.g., Bakke & Olsson 1986). Once the biofilm thickness has been determined, the value of $X_{\text{Tot,F}}$ can be directly calculated. For the biofilm thickness and the biomass concentration, typical values are provided in Table 2.

Sludge production (calibration step 1c)

Sludge production in the actual treatment plant and in model predictions should be compared. Large deviations may mean that sludge production in the treatment plant was measured incorrectly, particularly since biomass detachment from the biofilm carriers is a dynamic process requiring long-term sampling to achieve representative values. Another source of deviations between modeling results and observed reactor operation is an error in the wastewater characterization (e.g., inert particulate organic matter) or neglecting S_B in the effluent. COD mass balancing and evaluation of oxygen input (aeration) can be used to verify the measured sludge production (Rieger *et al.* 2013).

COD removal

Degradation of soluble biodegradable COD (calibration step 2)

The dominant parameter influencing the degradation of soluble biodegradable organic substrate (S_B) is the mass transfer boundary layer thickness (L_L), if biofilm thickness and concentration of biomass in the biofilm are fixed. Therefore, measured bulk phase S_B concentrations are compared with model predictions and calibrated by adjusting L_L . Typical values for L_L are provided in Table 3. Note that S_B should not be confused with the soluble COD measured in the reactor, as the soluble COD also includes the non-biodegradable soluble COD. In activated sludge modeling, particle characteristics (e.g., size) influence retention in a clarifier. In modeling a biofilm reactor, particle characteristics also influence attachment, retention, and potentially transport into the biofilm. Experimental procedures are available to differentiate between soluble, colloidal, and particulate COD (e.g., by measuring the filtered COD before or after flocculation. For details of wastewater characterization and an overview of related methods see Rieger *et al.* (2013)).

Note, as biofilm thickness and structure and mixing due to aeration may vary for different reactor stages, the value of

L_L can be significantly different for the different stages. As L_L is influenced by aeration intensity, the value of L_L will also change within a given stage for different air flow rates. One factor that can influence organic substrate degradation is the bulk-phase oxygen concentration, which should be measured and included. Another factor influencing organic substrate degradation is suspended heterotrophic biomass (e.g., from detached biomass). Even without selective retention of suspended biomass in the system, the effect of suspended biomass can be significant and should be considered experimentally (e.g., by measuring the removal rate of biofilm carriers after removing bulk phase biomass) and in the mathematical model.

Nitrogen removal

Nitrification (calibration step 3a)

Nitrification is significantly affected by the presence of heterotrophic growth (Wanner & Gujer 1985), which means that model predictions of nitrification can be realistic only if degradation of organic carbon and growth of heterotrophic bacteria are modeled correctly (calibration step 2). Nitrification in the actual plant should be evaluated based on measurements of organic nitrogen, NH_4^+ , NO_2^- , and NO_3^- . In many practical cases, only NH_4^+ and NO_3^- are measured, resulting in significant uncertainty in quantifying the actual extent of nitrification. Measured nitrification rates and nitrogen compounds can be compared with model predictions and, like in calibration step 2, the rate of ammonia oxidation can be adjusted by adjusting the value of L_L in the appropriate stages.

Potential pitfalls that should be considered when modeling nitrification are as follows:

- Ammonification of organic nitrogen may be limited in biofilm reactors due to low HRT.
- Nitrification may be limited by low pH (models usually monitor alkalinity as proxy for pH), low phosphorus concentrations, or by the presence of inhibitory compounds (check for these limitations both in the model and in the real plant).
- The number of layers in the mathematical model may have a significant influence on model predictions as it influences how competition between heterotrophic and autotrophic bacteria is modeled.

If in doubt, it may be worth the effort to sample biofilm carriers and measure nitrification and oxygen uptake rates in batch experiments after adding ammonium (no organic carbon) under different operating conditions (variation of

Table 2 | Reasonable parameter values for the concentration of biomass in the biofilm, biofilm thickness, and oxygen transfer to serve as a plausibility check for measured or calibrated values

		Carbon oxidation	Nitrification	Tertiary denitrification with methanol	Denitrification on membrane with H₂
Concentration of biomass in the biofilm ($X_{Tot,F}$), g VSS/L of biofilm		20–30	40–60	40–60	40–60
Biofilm thickness (L_F), μm	Trickling filter	500 (Top of trickling filter) 100 (Low loaded bottom)	100–200 (Top of trickling filter) 20–40 (Low loaded bottom)	Like for carbon oxidation, but perhaps with streamers	
	RBC	500 (First section) 100 (Low loaded last section)	100–200 (First section) 20–40 (Low loaded last section)		
	BAF (dense media)	100 (before backwashing) 40–60 (after backwashing)	20–40		
	BAF (floating media)	100–200	80–120		
	MBBR	500	100–200		
	MBfR (membrane biofilm reactor)				20–80
	Continuous washed sand filter (Dynasand)			10–20 No streamers	
	Fluidized bed reactors		10–20	40–50	
D_F		$= 0.8 \cdot D$			
Ratio of the wastewater to clean water oxygen mass transfer coefficient: α	BAF	1			
	MBBR	0.5–0.9			
	IFAS	Like for activated sludge, but media may influence the value			

Table 3 | Typical parameter values for flow, carrier sizes, and the external mass transfer boundary layer thickness (L_L) to serve as a plausibility check for measured or calibrated values

Type of reactor	Liquid velocity in m/h	Carrier size in mm	L_L in μm
Slow sand filter	0.04	0.6	100
Rapid sand filter	5	0.7	20
Trickling filter (low rate)	0.08	40	1,500
Trickling filter (high rate)	1.7	40	20
Submerged biofilm reactor	2–10	2–6	100
MBBR	a	b	50–180
UASB reactor	1	3	200
Fluidized bed	33	1	20

^aNot applicable. ^bVariable geometries as described in McQuarrie & Boltz (2011); sources: Kissel (1986), Morgenroth (2008).

oxygen set point and/or mixing intensity) to clearly identify what is limiting nitrification. Other comments regarding the calibration of L_L from calibration step 2, such as the influence of air flow rates on L_L , should be considered.

Denitrification (calibration step 3b)

Realistic calibration of denitrification relies on reliable measurements of all nitrogen species, including NO_3^- , NO_2^- , NH_4^+ , and organic nitrogen (in particulate organic matter and from biomass synthesis). Modeled denitrification rates depend on a range of different factors that need to be adjusted based on understanding of the actual reactor system:

- Availability of competing electron acceptors (e.g., DO).
- Availability of soluble organic carbon (S_B) or storage products (e.g., PHA) as electron donor and hydrolysis of colloidal or particulate organic carbon in the stage where denitrification occurs.
- External boundary layer thickness (L_L) in the stage where denitrification occurs. Again, note that the value of L_L in this stage will most likely be larger compared to reactors with more mixing due to intensive aeration.
- As for nitrification, choosing the right number of layers for the model is crucial for modeling simultaneous nitrification and denitrification.

Aeration

Modeling aeration, gas transfer, and oxygen transfer between stages (calibration step 4)

Biofilm reactors usually are mass-transfer limited, and oxygen often is the limiting factor for carbon oxidation

and nitrification, and can inhibit denitrification. Therefore, overall model predictions will be very sensitive to correctly modeling the availability of oxygen. Different approaches are available. If a particular stage in the real plant is operated with a set point for bulk-phase oxygen, then such a fixed bulk-phase concentration should also be implemented in the model. For reactors without aeration the bulk-phase oxygen concentration should not simply be set to zero, as oxygen may enter from recycles from other reactors in addition to transfer from the atmosphere. Thus, bulk-phase oxygen concentrations should always be modeled as a state variable rather than simply assuming a fixed value.

As noted in the previous calibration steps, air flow influences mixing intensity and indirectly the values of L_L in the different stages. That means that it would be desirable to develop an empirical correlation between oxygen transfer and gas flow (i.e., $k_L a$ and α values) and, in addition, to develop an empirical correlation between the gas flow and L_L .

Some typical pitfalls and suggestions

- Reactor hydraulics of full-scale plants in general are quite different from pilot plants or from the original design assumptions made, e.g., an assumed completely mixed reactor may in reality be semi-plug flow.
- The model utilized might not be applicable to the problem: e.g., biological phosphorus removal is taking place in the bulk phase of an IFAS, which requires that ASM2d be used for this aspect.
- The calibration steps outlined above do not always proceed in a linear manner. For example, calibration of aeration processes may affect earlier steps that involve DO limitation. Therefore, the entire process may need to proceed in an iterative manner.

CONCLUSIONS AND SUMMARY

A wide range of biofilm models and modeling platforms are available. A researcher or practitioner can take advantage of biofilm modeling to gain insight into what controls the performance of a process and for optimizing performance. A critical first step is choosing a model that has the appropriate level of complexity in terms of components and dimensionality. A good strategy is to choose the simplest model that includes the necessary components. In most cases, a 1D biofilm model will work best, and good choices are available for 1D modeling. They can range from hand-calculation analytical solutions, simple spreadsheets, and numerical-method platforms.

We present a five-step framework for good practice in biofilm reactor modeling (GBRMP). The first four steps are: (1) obtain information on the biofilm reactor system, (2) characterize the influent, (3) choose the plant and biofilm model, and (4) define the conversion processes. Each of these steps demands that the model user understands the most important components and features of the system. Establishing this kind of disciplined thinking is one of the main benefits of doing biofilm modeling.

The fifth step is to calibrate the model: System-specific model parameters are adjusted within reasonable ranges so that model outputs match actual system performance. Calibration is not a simple 'by the numbers' process, and it requires that the modeler follows a logical hierarchy of steps. Calibration requires that the modeler uses sound judgment about which parameters are system specific and open to calibration. It also requires that the adjusted parameters remain within realistic bounds and that the calibration process be carried out in an iterative manner.

Once each of steps 1 through 5 is completed satisfactorily, the calibrated model can be used for its intended purpose, such as optimizing performance, trouble-shooting poor performance, or gaining deeper understanding of what controls process performance.

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