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Low model order approximations of continuously stirred biofilm reactors with Monod kinetics

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Abstract

Design of controllers and optimization of plants using biofilm reactors require dynamic models and efficient methods of simulation. Continuously stirred biofilm reactors (CSBRs) are useful model units in modeling a variety of different types of biofilm reactors. Often the reaction kinetics in the biofilm is described by a Monod expression. With standard modeling assumptions the equations describing the fast dynamics of a CSBR will then, for each substrate, be one nonlinear partial differential equation coupled with one linear ordinary differential equation. Here, it is shown how a few nonlinear ordinary first order differential equations, which may be solved with standard integration methods, can be used as a close approximation for both dynamic responses and steady state solutions. These low order models can conveniently be used in simulation software and for controller design.

Keywords: Biofilms; Bioreactors; Control; Dynamic modeling; Dynamic simulation; Wastewater treatment

1. Introduction

A biofilm can be characterized as an organic matrix consisting of a complex community of bacteria, algae, fungi and protozoa embedded in organic polymers. In fixed biofilm reactors the biofilm is attached to substrata that, generally, are impermeable. Substrates diffuse from the bulk liquid into the biofilm where the bacteria carry out the desired transformations of the substrates. For different kinds of biofilm reactors, the biofilm substrata may be suspended carrier material or fixed packing media that can be either structured or random. Typical examples of fixed biofilm reactors are: biological fluidized beds, biofilters of different kinds, moving bed reactors, rotating biological contactors, and trickling filters. Reactors of this kind have attained increased attention during the last three decades, particularly in drinking water and wastewater treatment, due to the ability to withhold bacterial populations having low growth rates, and new materials that give high specific capacities [1,2].

To increase the knowledge about the dynamics of biofilm reactors, modeling is an important tool, but the detailed models that arise are often very complex. Mathematically, they are systems of stiff nonlinear partial differential equations with a moving boundary (the biofilm thickness). For optimization, controller design and for studies of large complex systems the mathematical models have to be neither detailed nor extremely accurate. However, the models have to be dynamic if, for example, they are to be used in controller design [3].

One simplification that can be made is to divide the dynamics of biofilm reactors into slow modes and fast modes. The fast dynamics are mainly caused by the reactor hydraulics and diffusive mass transfer in the biofilm, while the slow dynamics are caused by the growth and decay of the organisms in the biofilm. These dynamic modes are generally separated by several orders of magnitude since it, generally, takes days for the fauna to change while the fast transients settle in less than an hour [4]. Thus, the slow transients can often be ignored when only the fast dynamics are studied.

Most of the reported dynamic modeling and work on biofilm reactors have been focused on the slow biofilm dynamics, which have effects on the operation of the plants over longer periods of time [5–7]. However, there are several reasons to investigate, to model and to analyze the fast dynamics also. First of all, in the daily operation of a plant using biofilm reactors, the fast dynamics should be taken into considera-

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tion when optimizing the operation, and to guarantee stable control systems. The fast dynamics also play an important role for the reactor efficiency when the substrate load varies quickly [8]. Further, since physically based models of the fast dynamics are in many ways simplifications of more complex models of the slow dynamics, important model parameters are the same [4,9,10]. Hence, parameter identification from experimental data, using models of the fast dynamics, can be a way of acquiring information about the slow dynamics as well [11,2].

A continuously stirred biofilm reactor (CSBR) can be defined as an ideally stirred tank reactor, where the reactions take place in a biofilm attached to an impermeable substratum. The reaction kinetics in the biofilm is generally nonlinear. With standard modeling assumptions (see the next section), the equations describing the fast dynamics of a CSBR are, for each substrate, one nonlinear partial differential equation (PDE) coupled with one linear ordinary differential equation (ODE) for the mixing in the bulk:

$$V\frac{\mathrm{d}}{\mathrm{d}t}\tilde{S}^{\mathrm{b}} = Q(\tilde{S}^{\mathrm{b}}_{\mathrm{in}} - \tilde{S}^{\mathrm{b}}) - AD\frac{\partial \tilde{S}}{\partial \tilde{x}}\bigg|_{\tilde{x}=L} \tag{1}$$

$$\varepsilon\frac{\partial \tilde{S}}{\partial t} = D\frac{\partial^2 \tilde{S}}{\partial \tilde{x}^2} - r(\tilde{S}), \quad 0 < \tilde{x} < L \tag{2}$$

with boundary conditions

$$\tilde{x} = 0: \quad \frac{\partial \tilde{S}}{\partial \tilde{x}} = 0 \tag{3}$$

$$\tilde{x} = L: \quad \begin{cases} S = \tilde{S}^{\mathrm{b}} & \text{Dirichlet condition or} \\ \dfrac{\partial \tilde{S}}{\partial x} = \dfrac{D}{L_{\mathrm{w}}}(\tilde{S}^{\mathrm{b}} - \tilde{S}) & \text{Mixed condition,} \end{cases} \tag{4}$$

where $\tilde{S}$ is the substrate concentration in the biofilm, $\tilde{S}^{\mathrm{b}}$ the bulk concentration and $\tilde{x}$ is the distance from the substratum. Here, A is the total area of biofilm in the CSBR, V the bulk volume, Q the flow through the reactor, D the diffusion constant, L_{w} the thickness of a liquid boundary layer and L denotes the biofilm thickness. The void fraction in the biofilm is denoted ε and r is the substrate uptake rate by bacteria. In this formulation S can be a vector of substrates though, in the work presented here, we only consider one substrate. However, the derived approximations are directly applicable to cases with several substrates when the kinetics is independent of each other, and if there is only one reaction and stoichiometric relations between the substrates the same method to derive the approximations can be used.

The most straightforward solution to Eqs. (1) and (2) is to discretize both equations in time and approximate the space derivative in Eq. (2) with finite differences, for example. Alternatively, the equations can be solved using the finite element method. However, these approaches require a fine discretization of the biofilm due to the large spatial variations of the substrate concentration inside the biofilm. For many process-engineering purposes, such as system simulation and controller design, this makes the calculations too demanding or the model of too high order. Since the main interest in these cases is the input/output behavior of the bulk concentrations, and not a detailed description of the biofilm itself, there is room for model reduction.

When the reaction rate r depends linearly on the substrate concentration and the system is in a steady state, the equations can be solved analytically. Wik and Breitholtz [11] have studied the dynamic case when the reaction rate can be assumed to depend linearly on the substrate concentration. They derived a residue method that closely approximates the input/output behavior with only two linear first order ODEs. A comparison with other methods revealed that the Galerkin method in many cases also resulted in close approximations with only a few first order ODEs. These results have been extended to the case when two substrates are involved in the kinetics [12].

The most common kinetics for biological substrate uptake is the Monod expression

$$r = \mu_{\mathrm{m}}\frac{X}{Y}\frac{\tilde{S}}{\tilde{S} + K_{\mathrm{s}}}, \tag{5}$$

where μ_{m} is the maximum growth rate, X the bacterial concentration, Y the yield coefficient, K_{s} the saturation coefficient and $\tilde{S}$ is the substrate concentration. For very low ($\tilde{S} \ll K_{\mathrm{s}}$) and very high substrate concentrations ($\tilde{S} \gg K_{\mathrm{s}}$) linear kinetics can be assumed and the methods referred to above [11,12] apply, but in many cases the nonlinear kinetics has to be used [13]. For the steady state nonlinear case Sáez and Rittman [14] have developed a pseudo-analytical steady state solution, which is still the most widespread method used. However, for the nonlinear dynamic case that is the focus of this study no simple and low order model is available in the literature.

We see that the Monod expression is only mildly nonlinear in substrate concentration. It is therefore reasonable to believe that it should be possible to use only a few ODEs to approximate the system in a similar manner as in the linear cases [11]. Indeed, we will show how a few nonlinear first order ODEs, which may be solved with standard integration methods, can be used as a sufficiently close approximation for the nonlinear case. The suggested approximation is achieved using the orthogonal collocation method after comparison with other Methods of Weighted Residuals[1] (MWR), such as the Galerkin and the subdomain methods (see e.g. [15]). All approximations are evaluated by comparison with simulations, using a high accuracy finite element method (FEM), of step responses and responses to random influent concentrations. These comparisons show that for many parameter combinations the approximations are very accurate, making it possible to use only a second order state space model to approximate the system. Such low order models are suitable for controller design, stability analysis and simulation and optimization of systems having biofilm reactors.

[1] In MWR, an approximate solution to the PDE is forced to satisfy the boundary conditions and inserted into the PDE, hence creating a residual (error). The residual is multiplied by weights, integrated with respect to space over the region of definition, and then set to zero. This creates a finite dimensional (ODE) description of the infinite dimensional (PDE) model.

Examples of control applications where the approximations are directly applicable are when the reactor effluent concentration is controlled to follow a reference or setpoint by manipulating the influent load. This can either be achieved by varying the flow around an operating point or by changing the feed blend, such as in the addition of highly concentrated reject water from activated sludge presses to nitrifying reactors or the addition of an external carbon source to denitrifying biofilm reactors. In the former case a slightly modified definition of influent concentration has to be used [11,12].

The stationary solution of the approximations can either be used as they are or to generate initial values for dynamic simulations or for iterative methods to find stationary solutions of more complicated models used in, for example, simulations of the slow bacterial dynamics. A comparison with the pseudo-analytical solution by Sáez and Rittman [14], shows that the stationary approximations presented here are comparable and even better for many common parameter combinations, though less accurate for others. Note, however that the steady state approximation method proposed here have the advantage of being directly compatible with the dynamic approximations. It also gives an estimated concentration profile inside film, which can be used when the model is combined with biological models [16,17] and is also illustrative for educational purposes [18].

2. Material and methods

We model a CSBR as a continuously stirred tank with bulk volume V through which there is a flow Q of bulk liquid. The influent substrate concentration is $\tilde{S}^{\mathrm{b}}_{\mathrm{in}}$ and the effluent concentration, which equals that in the bulk of the CSBR, is $\tilde{S}^{\mathrm{b}}$. The substrate diffuses without transfer resistance into a biofilm where the reactions take place, i.e. the Dirichlet condition in Eq. (4) is used as boundary condition at the biofilm surface. The substrate concentration ($\tilde{S}$) is assumed to be continuous in time ($\tilde{t}$) and space ($\tilde{x}$). Further, the void fraction (ε) in the biofilm, the substrate diffusion coefficient (D), and the thickness of the biofilm are assumed constant. If the biofilm is homogeneous and the transport of substrates inside the biofilm obeys Fick's law of diffusion in one dimension, a CSBR is described by Eqs. (1) and (2) in dimensionless form. These equations can be written,

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} S^{\mathrm{b}} = S^{\mathrm{b}}_{\mathrm{in}} - S^{\mathrm{b}} - \gamma \left.\frac{\partial S}{\partial x}\right|_{x=1} \tag{6}$$

$$\frac{\partial S}{\partial t} = \frac{\partial^2 S}{\partial x^2} - \alpha \frac{S}{S+1}, \quad 0 < x < 1 \tag{7}$$

$$x = 0: \quad \frac{\partial s}{\partial x} = 0; \qquad x = 1: \quad S = S^{\mathrm{b}}, \tag{8}$$

where the substrate concentration has been scaled to $S^{\mathrm{b}} = \tilde{S}^{\mathrm{b}}/K_{\mathrm{s}}$ and $S = \tilde{S}/K_{\mathrm{s}}$, $\tau = VD/(QL^2\varepsilon)$, $\gamma = AD/QL$ and $\alpha = L^2\mu_{\mathrm{m}}X/(K_{\mathrm{s}}DY)$. Space and time are scaled as $x = \tilde{x}/L$ and $t = \lambda\tilde{t}$, where $\lambda = D/(L^2\varepsilon)$.

We now extend the mass balance (7) to $-1 < x < 1$. The boundary conditions (8) then imply that the solution must be symmetric around $x = 0$. We can therefore approximate the substrate concentration inside the biofilm with a trial function of even polynomials,

$$\hat{S}(t, x) = \sum_{k=0}^{m} \theta_k(t) P_{2k}(x), \tag{9}$$

where P_{2k} are Legendre polynomials of order $2k$ (symmetric), orthogonal on $-1 \le x \le 1$ and normed such that $P_{2k}(1) = 1$. The approximate bulk concentration we get by using this approximation in Eq. (6) is denoted $\hat{S}^{\mathrm{b}}$. The next step of the MWR method is to set the weighted residuals of Eq. (7) to zero, i.e. setting

$$\int_{-1}^{1} W_n(x) \left(\frac{\partial \hat{S}}{\partial t} - \frac{\partial^2 \hat{S}}{\partial x^2} + \alpha \frac{\hat{S}}{\hat{S}+1} \right) \mathrm{d}x = 0,$$
$$n = 0, 1, \ldots, m \tag{10}$$

where $W_n(x)$ is a weight function that depends on the choice of MWR method. For the orthogonal collocation method $W_n(x) = \delta(x - x_n)$, where x_n are the zeros of a Jacobi polynomial, while for the Galerkin method $W_n(x) = P_{2n}(x)$. In the subdomain method, the region of definition for the PDE is divided into a number of smaller regions (subdomains). The weights are chosen to be unity on each subdomain and zero everywhere else, i.e. the integrated residual is set to zero on each subdomain. In this study, the best approximation turns out to be the one achieved by the orthogonal collocation method, which is therefore described more in detail.

Forcing the approximation to satisfy the boundary condition $\hat{S}(1, t) = \hat{S}^{\mathrm{b}}$, setting the residuals of Eq. (7) to zero at $m+1$ points, i.e. using $W_n(x) = \delta(x - x_n)$ in Eq. (10) and inserting the approximation $\hat{S}$ into Eqs. (6) and (10) give

$$\sum_{k=0}^{m} \theta_k = \hat{S}^{\mathrm{b}} \tag{11}$$

$$0 = \sum_{k=0}^{m} \left\{ P_{2k}(x_j) \frac{\mathrm{d}}{\mathrm{d}t} \theta_k - \theta_k \left.\frac{\mathrm{d}^2 P_{2k}}{\mathrm{d}x^2}\right|_{x=x_j} \right\} + \alpha \frac{\sum_{k=0}^{m} \theta_k P_{2k}(x_j)}{1 + \sum_{k=0}^{m} \theta_k P_{2k}(x_j)}, \quad j = 1, 2, \ldots, m+1 \tag{12}$$

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \hat{S}^{\mathrm{b}} = S^{\mathrm{b}}_{\mathrm{in}} - \hat{S}^{\mathrm{b}} - \gamma \sum_{k=0}^{m} \theta_k \left.\frac{\mathrm{d}P_{2k}}{\mathrm{d}x}\right|_{x=1} \tag{13}$$

where $\hat{S}^{\mathrm{b}}$, $\hat{S}$, $\hat{S}^{\mathrm{b}}_{\mathrm{in}}$ and θ_k are functions of time t.

The algebraic equation (11) is used to eliminate one of the differential equations in (12). This means that we only need m collocation points. In this case, the m collocation points are chosen as the positive roots of the Legendre polynomial P_{2m}, which is a special case of Jacobi polynomials. The resulting

state space model can then be written as

$$\sum_{k=0}^{m-1}\frac{\mathrm{d}}{\mathrm{d}t}\theta_k P_{2k}(x_j) = \sum_{k=0}^{m-1}\theta_k\left(\frac{\mathrm{d}^2P_{2k}}{\mathrm{d}x^2}-\frac{\mathrm{d}^2P_{2m}}{\mathrm{d}x^2}\right)\Bigg|_{x=x_j} + \hat{S}^{\mathrm{b}}\frac{\mathrm{d}^2P_{2m}}{\mathrm{d}x^2}\Bigg|_{x=x_j} - \alpha\left(\frac{\sum_{k=0}^{m-1}\theta_k P_{2k}(x_j)}{1+\sum_{k=0}^{m-1}\theta_k P_{2k}(x_j)}\right), \quad j=1,2,\ldots,m \tag{14}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{S}^{\mathrm{b}} = \frac{1}{\tau}(S_{\mathrm{in}}^{\mathrm{b}}-\hat{S}^{\mathrm{b}}) - \frac{\gamma}{T}\left(\sum_{k=0}^{m-1}\theta_k\left(\frac{\mathrm{d}P_{2k}}{\mathrm{d}x}-\frac{\mathrm{d}P_{2m}}{\mathrm{d}x}\right)\Bigg|_{x=1} + \hat{S}^{\mathrm{b}}\frac{\mathrm{d}P_{2m}}{\mathrm{d}x}\Bigg|_{x=1}\right) \tag{15}$$

For $m=1$, the state space model can be written as

$$\begin{cases}\dfrac{\mathrm{d}}{\mathrm{d}t}\theta_0 = 3(\hat{S}^{\mathrm{b}}-\theta_0) - \dfrac{\alpha\theta_0}{1+\theta_0}\\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{S}^{\mathrm{b}} = \dfrac{1}{\tau}(S_{\mathrm{in}}^{\mathrm{b}}-(1+3\gamma)\hat{S}^{\mathrm{b}}+3\gamma\theta_0)\end{cases} \tag{16}$$

The stationary solution is determined by setting the time derivatives of the above equations to zero.

If we use $y=(S_{\mathrm{in}}^{\mathrm{b}}-S^{\mathrm{b}})/2\gamma$ the steady state for $m=1$ is given by

$$f(y) = 2y-\alpha\left(1-\frac{3}{3(1+S_{\mathrm{in}}^{\mathrm{b}})-2(1+3\gamma)y}\right) = 0. \tag{17}$$

After solving for y, the stationary bulk concentration and the concentration in the biofilm follows from

$$S^{\mathrm{b}} = S_{\mathrm{in}}^{\mathrm{b}} - 2\gamma y \tag{18}$$

$$S(x) = S_{\mathrm{in}}^{\mathrm{b}} - (1+2\gamma)y + x^2 y. \tag{19}$$

Expanding to $m=2$, the state space model can be written as

$$\begin{cases}\dfrac{\mathrm{d}}{\mathrm{d}t}\theta_0 = 10(\hat{S}^{\mathrm{b}}-\theta_0)-7\theta_1+\alpha\left(-1+\dfrac{0.6521}{1+\theta_0-0.3266\theta_1}+\dfrac{0.3479}{1+\theta_0+0.6123\theta_1}\right)\\ \dfrac{\mathrm{d}}{\mathrm{d}t}\theta_1 = 35(\hat{S}^{\mathrm{b}}-\theta_0-\theta_1)+\alpha\left(-\dfrac{1.0652}{1+\theta_0-0.3266\theta_1}+\dfrac{1.0652}{1+\theta_0+0.6123\theta_1}\right)\\ \dfrac{\mathrm{d}}{\mathrm{d}t}\hat{S}^{\mathrm{b}} = \dfrac{1}{\tau}(S_{\mathrm{in}}^{\mathrm{b}}-(1+10\gamma)\hat{S}^{\mathrm{b}}+10\gamma\theta_0+7\gamma\theta_1)\end{cases} \tag{20}$$

Also for $m=2$, it is possible to derive one single equation for the steady state solution.

To estimate the approximation errors the MWR approximations are compared to high accuracy FEM solutions. The FEM simulations were carried out in the software MATLAB (The Mathworks Inc., Natick, MA, USA) using the toolbox FEMLAB (Comsol Inc., Burlington, MA, USA). For the FEM solver the absolute tolerance was set to 10^{-5} and the relative tolerance to $\tau\times10^{-4}$ when $\tau<1$ and otherwise 10^{-4}. The number of node points were 305 with increasing density towards $x=1$. This was done by initializing a mesh by setting the maximum general element size to 1/120, the maximum element size near the vertex $x=1$ to 1/4000 and the mesh growth rate to 1.3. The mesh was then refined once. The rest of the solver settings had default values.

The accuracy of the numerical results from the FEM calculations was verified by decreasing the number of node points to half and also by increasing the absolute and relative tolerance to 10^{-4} and 10^{-3} (or $\tau\times10^{-3}$). This had negligible effects on the numerical results. As an example, the average error between the FEM solution calculated with these conditions and the FEM solution used in comparison with the MWR approximations was less than 0.001% for a unit step response when $\alpha=300$, $\gamma=3$ and $\tau/\gamma=10$, the most difficult parameter combination investigated.

In a steady state, the ODE (6) can be eliminated and the PDE (7) can be solved using FEMLAB in a quite straightforward manner. The calculations are fast compared to the dynamic simulations and the error tolerances can be set to a value as low as 10^{-8}.

To find the steady state approximations the equations were solved using the MATLAB function *fsolve*. The tolerance was set to the same value as for the FEM solution, i.e. 10^{-8}. Also the dynamic simulations of the approximations were carried out in MATLAB, using one of the built in ODE solvers for stiff differential equations (*ode23s*). The error tolerances were set to the same values as for the FEM simulation. The computational time for simulating the approximations were small. For example, the simulation time for a simple step response with $m=2$ was about 0.3 s on a Dell PC with Intel(R) Pentium(R) 4 CPU 2.00 GHz processor. This should be compared to a FEM simulation time of about 3 min.

The simulations were carried out for a number of different combinations of the three model parameters α, γ and τ. The parameter intervals were determined by calculating typical parameter values for different types of reactors and biofilms using the expressions for α, γ and τ. From a parameter point of view two extremes of reactor types are trickling filters, with a very small ratio of bulk water volume (V) to water volume contained in the biofilm (εAL), and moving beds, which have a very large ratio. In terms of biofilms, we have autotrophic biofilms with slow growth (substrate uptake rate) and thin biofilm, heterotrophic aerobic films with rapid growth and thick films, and anoxic heterotrophic films that can be thick though with a less rapid growth. The values presented here are example values for these biofilms and reactor types (see Table 1).

Table 1
Model parameters

Substrate		Aerobic growth autotrophs				Aerobic growth heterotrophs		Anoxic growth heterotrophs	
		NH_4	O_2	Alk	NO_2	COD	O_2	COD	NO_x
High rate trickling filters	α	0.12	0.87	0.06	0.33	28	272	18	64
	γ	0.25	0.29	0.15	0.22	0.14	0.29	0.14	0.22
	τ	0.49	0.58	0.30	0.44	0.03	0.07	0.03	0.06
	$\frac{\tau}{\gamma}$	2.00	2.00	2.00	2.00	0.25	0.25	0.25	0.25
Moving bed bioreactors	α	0.01	0.010	0.006	0.04	16	153	10	36
	γ	10	12	6	9	0.35	0.73	0.35	0.56
	τ	493	580	303	443	0.95	1.98	0.95	1.52
	$\frac{\tau}{\gamma}$	48	48	48	48	2.7	2.7	2.7	2.7

The dynamic simulations were run for all combinations of $\alpha = 0.003$, 0.03, 1, 30 and 300; $\gamma = 0.1$, 0.33, 1, 3 and 10; $\tau/\gamma = 0.02$, 0.1, 1, 10 and 50.

These combinations gave a total of 125 simulations covering typical cases for all the considered biofilms and reactors. The Monod expression used to describe the substrate uptake rate is approximately linear at both high and low substrate concentrations. The maximum nonlinearity occurs for concentrations around $S = 1$, which was the influent concentration S^b_{in} chosen for all the dynamic simulations. The stationary solution was calculated for $S^b_{in} = 0.1$, 1, 10 and the values of α and γ presented above (the value of τ does not affect the steady state).

To estimate the approximation error, the MWR approximation and a FEM solution were compared. For the steady state simulations, the relative error was calculated according to

$$e_{rel} = \frac{|\hat{S}^b - S^b_{FEM}|}{S^b_{FEM}}, \tag{21}$$

where S^b_{FEM} is the FEM solution and $\hat{S}^b$ is the MWR solution.

As a measure of accuracy of the dynamic step responses, the relative error was calculated as

$$e_{rel} = \frac{\int_0^{5T} |S^b_{FEM} - \hat{S}^b| \, dt}{\int_0^{5T} S^b_{FEM} \, dt}, \tag{22}$$

where T is the scaled characteristic time $\tilde{T} = (V + \varepsilon AL)/Q$ (corresponds to $T = \tau + \gamma$). The integrals were evaluated by quadrature using the MATLAB function *quad*.

To evaluate how the system responds to an arbitrary input, the response to a low pass filtered random signal was simulated. The time scale for each parameter combination was scaled by the characteristic time of the system (see Fig. 1). Again, the average error was calculated as in Eq. (22) but integrated over the entire input interval.

3. Results

3.1. Steady-state models

Fig. 2 shows the relative error for the second order ($m = 1$) approximation (16) and the third order ($m = 2$) approximation (20), as well as the pseudo-analytical method [14]. For $\alpha < 1$, the error is negligible ($e_{rel} < 10^{-4}$) for both $m = 1$ and $m = 2$.

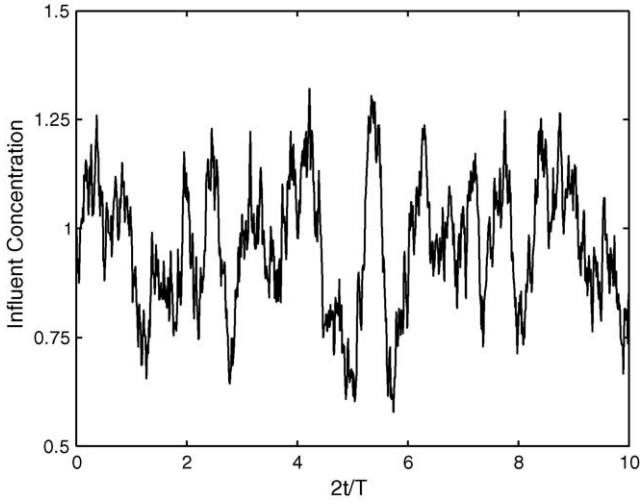

Fig. 1. Random input concentration used for evaluation.

Increasing γ increases the relative error for a given α. For $\alpha > 1$, the error is significant when $m = 1$, though for $m = 2$ the relative error is small even for $\alpha = 30$. For $\alpha = 300$ higher order approximations are required. The pseudo-analytical solution, on the

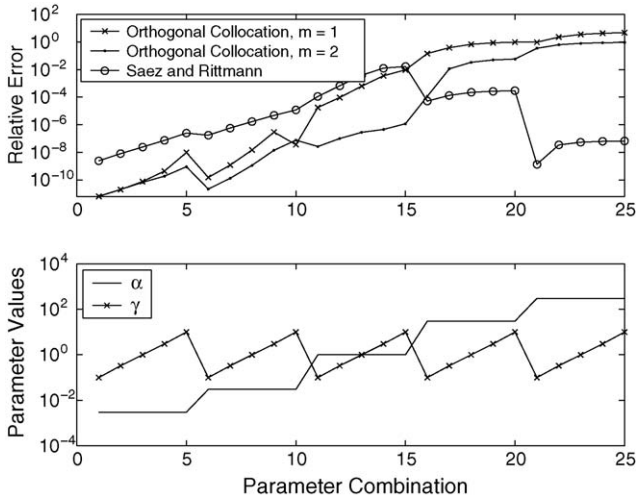

Fig. 2. Diagram showing a comparison of the pseudoanalytical solution by Sáez and Rittmann and the steady-state orthogonal collocation approximations for $S^b_{in} = 1$. Use bottom diagram to find the parameter combination from the biofilm reactor parameters α and γ.

other hand, is extremely accurate for the highest simulated values of α, but when $\alpha \leq 1$ even the lowest order approximations (16) in steady-state, i.e. (17), is more accurate.

Naturally, higher order approximations results in smaller errors. However, it takes a seventh order approximation to achieve a maximum error less than 0.1%, and a sixth order approximation to have a maximum error less than 1% for all parameter combinations. For $\alpha = 30$ it is more worthwhile to extend the state space model to a higher order. The maximum error when $m = 2$ is then 5.8%, while for $m = 3$ it is only 0.14%.

Fig. 3 shows the dependency on influent concentration. The errors decrease when S_{in}^{b} is increased. The dependency on the influent concentration for $m = 1$ is similar to that of $m = 2$.

3.2. Dynamic models

Fig. 4a shows the relative error (22) for the step responses of the orthogonal collocation approximation. For many parameter combinations the approximations are very accurate. When $m = 2$ and $\alpha \leq 1$ the errors are never more than 0.6%. If we also require τ not to be less than 0.1, the error is less than 0.05%. Smaller errors cannot be expected with the tolerances used. The error decreases with τ and increases with γ.

The second order ($m = 1$) approximation (16) is satisfactory for most applications when $\alpha \leq 1$. When $\alpha \leq 1$ and $\tau > 0.1$ the maximum error is 1.1%. Errors of the higher order approximations were also analyzed. The differences between the different order approximations are particularly significant when $\alpha \geq 1$.

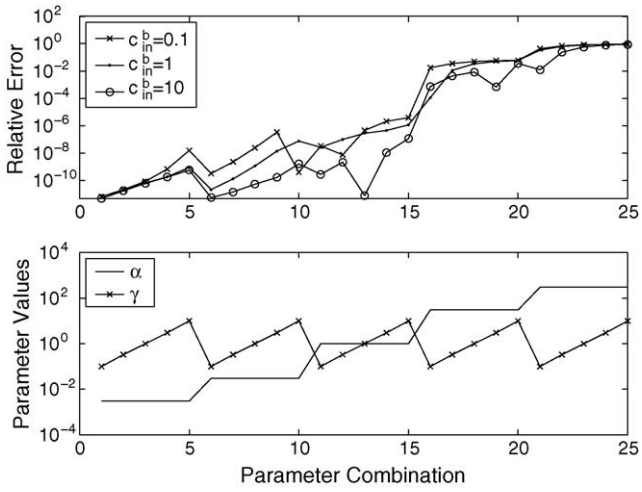

Fig. 3. Influent concentration dependency of the relative error for the steady-state orthogonal collocation method when $m = 2$. Use bottom diagram to find the parameter combination from the biofilm reactor parameters α and γ.

Fig. 4b shows the relative error for the response to the random influent concentration. The plot very much resembles that of a step response in that the large errors occur for the same parameter combinations. For the third order ($m = 2$) approximation (20) the errors are less than 1.8% when $\alpha \leq 1$.

For comparison, the results using the Galerkin approximation with $m = 2$ are also shown in Fig. 4b. As can be seen, the difference between the two approximation methods is negligible except for a few parameter combinations. The orthogonal col-

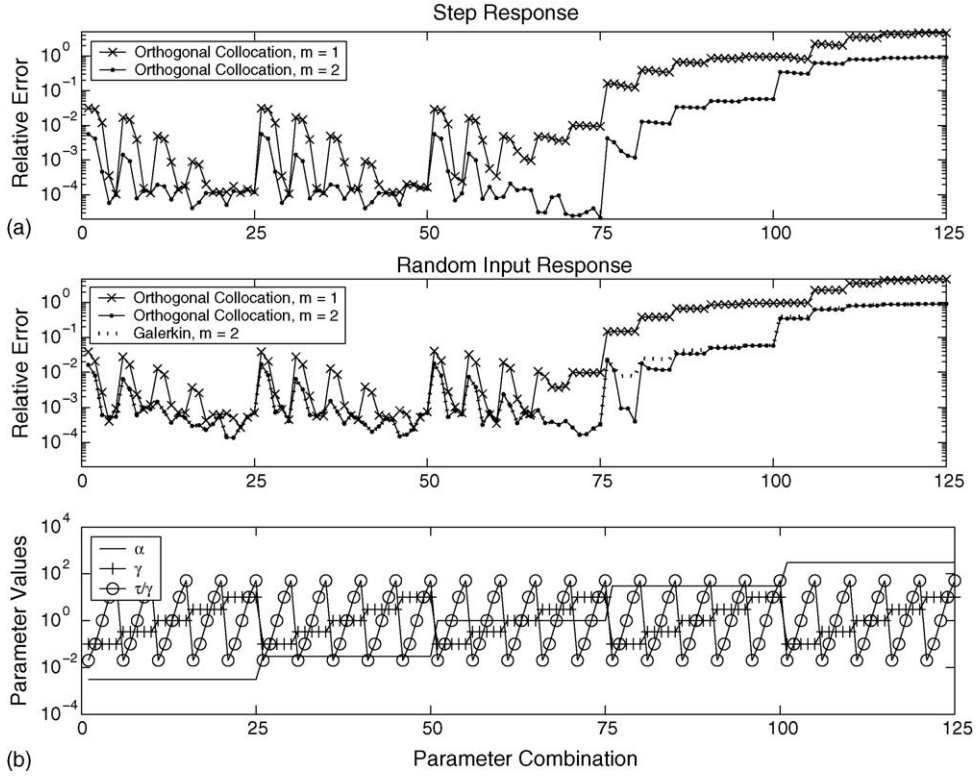

Fig. 4. (a) Relative error of the orthogonal collocation method for step responses. (b) Relative error of the orthogonal collocation method and the Galerkin method for responses to random influent concentrations. Use bottom diagram to find the parameter combination from the biofilm reactor parameters α, γ and τ (τ/γ).

Table 2
Number of collocation points (m) needed for unscaled model

	$e_{rel} < 1\%$	$e_{rel} < 3\%$	$e_{rel} < 10\%$
$\alpha \leq 0.03$	1	1	1
$\alpha \leq 1$	3	2	1
$\alpha \leq 30$	3	3	2
$\alpha \leq 300$	5	5	4

Table 3
Number of collocation points (m) needed for scaled model

	$e_{rel} < 1\%$	$e_{rel} < 3\%$	$e_{rel} < 10\%$
$\alpha \leq 0.03$	1	1	1
$\alpha \leq 1$	3	2	1
$\alpha \leq 30$	3	2	1
$\alpha \leq 300$	4	2	1

location method is actually slightly better where the errors are significant. The same conclusions could be drawn for $m = 1$ and also for the step response simulations.

Table 2 shows what model order is needed to get a maximum error less than 1, 3 and 10% for different values of α. The results from the random input responses are presented since these errors are over all somewhat higher than those from the step responses. The large errors for high values of α are clearly a consequence of the approximation steady state gain being inaccurate, as shown in Fig. 2.

The dynamic behavior, however, may still be satisfying. To be able to evaluate the dynamic behavior without the influence of the gain error, the step responses and the random input responses were divided by the steady state concentration at $c_{in}^{b} = 1$, and new errors were calculated. The results from these simulations show that the low order approximations describe the dynamic behavior of the system quite well. For $m = 1$, the maximum relative error is 6.8%. For most parameter combinations the error is significantly smaller. The corresponding number for the third order ($m = 2$) approximation is 2.8%. The largest errors still occur when $\alpha = 300$. Table 3 shows what model order is needed to get a maximum error less than 1, 3 and 10% for the scaled model.

4. Discussion

The orthogonal collocation method has the advantage of avoiding the integral calculation (10), which in this case becomes rather difficult for the Galerkin and subdomain methods as m grows large. Instead, the residual is evaluated at a number of discrete points. It can be shown that there is a strong connection between the optimal collocation method and the Galerkin method, which in general is regarded as the most accurate MWR approximation [19]. The subdomain method results in approximations that are very similar to the ones achieved in the Galerkin method and for $m = 1$ the methods are identical. In this paper, we have therefore concentrated on the approximations derived using the orthogonal collocation method. Galerkin and subdomain approximations have been simulated as well but since the results do not motivate the use of these approximations the results are not presented in detail here.

The results from steady-state simulations as well as dynamic simulations clearly show that the approximation error increases with α. This is not surprising since α is the factor that determines the emphasis of the nonlinear term in the biofilm Eq. (7). Obviously, it makes it harder to find a satisfying low order approximation for the model when α has a high value. Also, simulations with low values of τ will give larger errors than simulations with high values. The reason is that when τ is small the concentration in the biofilm, which is where the approximation take place, has more influence on the bulk concentration.

The stationary approximations can either be used as they are or to generate initial values for the dynamic approximations, or iterative methods to find stationary solutions of more complicated models used in, for example, simulations of the slow bacterial dynamics. A comparison with the pseudo-analytical steady state solution shows that the stationary approximations presented here are more accurate for $\alpha \leq 1$, but less accurate for high values of α. However, the approximations derived here have the advantage of being directly compatible with the dynamic model of the same order.

Simulations of step responses and responses to a random influent concentration show that a second order state space model is enough to describe systems with low reaction rates and large bulk volume compared to the biofilm liquid volume. This means that the ODE (6) and the PDE (7) are replaced by only two first order ODEs (16). However, as already mentioned, for high α-values (high reaction rates) or low values of τ (small ratio of bulk volume to biofilm void volume) the second order approximations are in many cases not accurate enough. For high values of α, it is mainly the stationary gain that is inaccurate. In such cases, if a low order approximation is desired, we recommend calculation of the steady state solution for the actual operating point with some other method, e.g. the pseudo-analytical solution, and a correction of the state space model by this stationary solution. Simulations of step responses and random input responses divided by the stationary gain give a maximum error of about 8% for the second order approximations and 3% for the third order approximations.

The third order state space models (20) are naturally better than the second order models, but they show the same dependency on the parameters. For high values of α and low values of τ the error grows very large. Which order approximation one should use is, of course, a matter of how accurate the solution needs to be. For the fifth order model the maximum error of the random input response is less than 5%, which would be accurate enough for most control applications. The maximum error of the sixth order model is as low as 0.5% and an approximation of that order should be sufficient in almost any application.

Examples of reactors for which the low order approximations are satisfying are reactors with aerobic growth of autotrophs, since for such biofilms $\alpha < 1$ and $\tau > 0.1$. If the reactor is a moving bed bioreactor ($\tau > 100$) even the lowest order approximation (16) is very accurate.

4.1. Uniqueness

Two properties of a nonlinear dynamic system are particularly important, i.e. stability of steady state operation (equilibrium points) and the uniqueness of such an operating point. Many bioreactors exhibit multiple steady states, i.e. depending on the initial conditions the system may end in different operating points for a given stationary operation. The question is therefore, does the CSBR system have multiple steady state or not, and does the approximation have the same property?

In a steady state, the time derivative is zero and we can solve Eq. (7) analytically with respect to dS/dx by integration from the biofilm substratum to the surface. Using Eq. (7) in a steady state, and denoting the first and second derivative of S by S' and S'', we have

$$\int_{x=0}^{1} S''S'\,dx = \alpha\int_{x=0}^{1}\left(1-\frac{1}{S+1}\right)S'\,dx = \alpha[S-\ln(S+1)]_{x=0}^{1}$$

Using the boundary conditions $S'(0)=0$ and $S(1)=S^b$ we also have $\int_0^1 S''S'\,dx = S'(1)^2/2$, which gives

$$\left.\frac{dS}{dx}\right|_{x=1} = \sqrt{2\alpha(S^b-S(0))-\alpha\ln\left(\frac{S^b+1}{S(0)+1}\right)}$$

Inserting this in Eq. (6) in a steady state gives

$$S_{in}^b - S^b - \gamma\sqrt{2\alpha(S^b-S(0))-\alpha\ln\left(\frac{S^b+1}{S(0)+1}\right)} = 0$$

or

$$\frac{(S_{in}^b-S^b)^2}{2\gamma^2\alpha} - S^b + \ln(S^b+1) = -S(0)+\ln(S(0)+1) < 0, \quad \forall S(0) > 0$$

The right hand side is strictly monotonically decreasing in $S(0)$ for all α and γ and, hence, for every stationary bulk concentration S^b and S_{in}^b there can only be one unique concentration $S(0)$ at the substratum. Now, given a $S(0)$ and the boundary condition $dS/dx=0$ at $x=0$ Eq. (7) can be regarded as an initial value problem

$$\frac{d}{dx}\begin{bmatrix} S(x) \\ S'(x)\end{bmatrix} = \begin{bmatrix} S'(x) \\ \alpha\dfrac{S(x)}{S(x)+1}\end{bmatrix},$$

which satisfies a Lipschitz condition with a Lipschitz constant $\sqrt{1+\alpha^2}$ (see e.g. [20]). This means that the initial value problem has a unique solution and, consequently, the CSBR system investigated here have only unique steady state solutions.

We will now show that all equilibrium points of the approximation (17) in the relevant interval are also unique, i.e. it is never possible to find more than one physically acceptable solution.

For the second order steady state approximation ($m=1$) the following should hold:

$$0 \le \hat{S}^b \le S_{in}^b \tag{23}$$

$$0 \le \hat{S}(0) = 1.5\theta_0 - 0.5\hat{S}^b \tag{24}$$

$$0 \le \left.\frac{d\hat{S}}{dx}\right|_{x=1} = 3(\hat{S}^b-\theta_0) \tag{25}$$

In a steady state, $\theta_0 = \hat{S}^b + (\hat{S}^b - S_{in}^b)/3\gamma$. With the inequalities above this implies that a physically realistic solution should be expected in the interval $S_{in}^b/(1+2\gamma) \le \hat{S}^b \le S_{in}^b$.

It can be shown that there is a unique steady state solution to Eq. (17) in the interval $(S_{in}^b - 3\gamma)/(1+3\gamma) < \bar{S}^b < S_{in}^b$. Notice that the expected interval is contained in this somewhat larger interval. According to Eq. (18) this interval translates into $0 < y < 3(1+S_{in}^b)/(2(1+3\gamma))$. Investigating Eq. (17) at the end points of this interval, we have

$$\lim_{y\to 0} f(y) = -\alpha\frac{S_{in}^b}{1+S_{in}^b} < 0$$

and

$$f(y)\to\infty, \quad \text{when} \quad y \to \frac{3(1+S_{in}^b)}{2(1+3\gamma)}.$$

Since $f(y)$ is a continuous function on the interval there exists, therefore, at least one solution to Eq. (17). The derivative of $f(y)$ is

$$\frac{d}{dy}f(y) = 2 + 3\alpha\left(\frac{2(1+3\gamma)}{(3(1+S_{in}^b)-2(1+3\gamma)y)^2}\right) > 0,$$

which is strictly positive. This implies that $f(y)$ is strictly monotonically increasing on the interval and, hence, the solution is unique.

4.2. Nonorthogonal collocation

Several comparisons with other MWR methods for different problems have shown that the orthogonal collocation approximation often is the most accurate and reliable collocation method [15,19]. In most of the studied cases, however, the purpose is to find an approximation of a single differential equation. In this case, we have two coupled equations and we are mainly interested in the bulk concentration, which is affected by the biofilm concentrations only by the concentration gradient at the biofilm surface. Hence, it is not obvious that the roots of orthogonal polynomials are the best choice of collocation points.

For the second order approximation ($m=1$) no collocation points are needed since the system is fully determined by the two boundary conditions. For higher order approximations the choice of collocation points may make a significant difference. A possibility is that the concentration gradient at the biofilm surface is best approximated by having collocation points near that surface. This was tested by simulating step responses for $m=2$ with collocation points $x_1=0.95$ and $x_2=0.99$. The orthogonal collocation method ($x_1\approx 0.34$ and $x_2\approx 0.86$) gave significantly better results, especially for $\alpha=1$. The combination of one collocation point near the surface $x_2=0.99$ and one in the middle of the biofilm $x=0.5$ showed again that orthogonal collocation is better.

Table 4
Influence of a liquid boundary layer on the relative error of a step response

	$\alpha=1, \gamma=0.1, \tau=0.1$	$\alpha=1, \gamma=0.33, \tau=0.33$
$m=1$		
$L_w=0.5L$	0.0032	0.0017
$L_w=0$	0.0110	0.0037
$m=2$		
$L_w=0.5L$	9.30×10^{-5}	3.80×10^{-5}
$L_w=0$	4.75×10^{-4}	7.57×10^{-5}

4.3. Diffusion layer on the biofilm surface

The simulations that have been presented so far do not take into account the effects of a boundary layer on the surface of the biofilm. If a boundary layer has developed, the boundary condition of the model becomes a mixed condition instead of a Dirichlet condition and the resulting approximations become somewhat modified. It is not obvious how this affect the accuracy of the approximations compared to the FEM solution. To get some idea about this, step response simulations were carried out for two different parameter combinations. In these simulations the model that takes the effect of a liquid boundary layer into account has been used, i.e. the mixed condition in Eq. (4) was taken as the boundary condition.

The thickness of the liquid layer, L_w, was supposed to be around half of the total bulk thickness V/A. For a high rate trickling filter with aerobic growth of autotrophs the bulk thickness is typically equal to the biofilm thickness, $V/A=L$. The values of α, γ and τ were chosen among those that have been used in the previous simulations and that are close to the typical values for a high rate trickling filter with aerobic growth of autotrophs. The following parameter combinations were chosen: $\alpha=1$, $\gamma=0.1$, $\tau=0.1$, and $\alpha=1$, $\gamma=0.33$, $\tau=0.33$.

In Table 4, the errors for the chosen parameter combinations are shown together with the errors calculated when the effect of the boundary layer was ignored, i.e. $L_w=0$. The results are unambiguous. The errors are at least halved when the effect of the boundary layer is considered. Hence, it is likely that the results derived in the previous sections can be applied to cases where a liquid boundary layer has developed. The reason for the higher accuracy in the case of a liquid boundary layer is probably the fact that the mixed boundary condition makes the ODE for the bulk and the PDE for the biofilm more weakly coupled.

5. Conclusion

Low order approximations describing the fast dynamics of continuously stirred biofilm reactors have been derived. The approximations were evaluated by comparison with high accuracy solutions derived with finite element method (FEM). Standard assumptions were made for the biofilm and Monod kinetics used to describe the substrate uptake rate. The resulting approximations are state space models consisting of only a few first order ODEs, which were derived using orthogonal collocation, see Eqs. (16) and (20). The orthogonal collocation method has a few advantages compared to other MWR methods, such as the Galerkin method. It gives simpler expression and in this case equal or higher accuracy.

It was shown that the system have only unique steady-state solutions.For the second order orthogonal collocation approximation it has been shown also the approximation has a unique steady state in a domain containing the domain where we expect the solution to be. This stationary solution can be found by solving one single equation. It was shown that the steady state approximations derived here are more accurate than the pseudo-analytical steady state solution by Sáez and Rittman [14] for $\alpha\leq1$ but less accurate for higher values of α. However, the approximations we suggest have the advantage of being directly compatible with the dynamic solution, which the pseudo-analytical method cannot be.

Simulations show that the second order state space model (16) is enough to describe systems with low reaction rates and large bulk volume compared to the biofilm liquid volume. An example of such a system is a moving bed bioreactor with aerobic growth of autotrophs. For high α-values (high reaction rates) or low values of τ (bulk volume small compared to biofilm liquid volume) the lowest order approximations are not accurate enough. The higher order the more accurate the approximation, but considering the relatively large uncertainties in biological systems, a model order of three is still enough for most cases. A sixth order approximation should be sufficient in almost any application. Which order of the approximation one should use depends on the desired accuracy. How many equations that are needed in the model to achieve a certain accuracy in the approximation is summarized in Tables 2 and 3.

For high values of α it is mainly the stationary gain that is inaccurate. If $\alpha\gg1$ and a low order approximation is desired, the steady state solution for the actual operating point should be calculated by some other method, e.g. the pseudo-analytical solution, and the state space model corrected by this stationary solution. The accuracy is then improved such that a second or third order model is sufficient for most control and simulation applications.

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