ADEQUATE COMPLEXITY FOR BIOFILM SYSTEMS MODELLING

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Introduction

The fact that makes biofilm models relatively complex is that not only the microbial conversion of substrate needs to be considered but also the diffusive transport of soluble substrates inside the biofilm. Recent advances in biofilm research (Bishop, 1997) conclude that the heterogeneity of the biofilm must be taken into account too. However, such detailed mathematical description of the processes in biofilms also has some shortcomings. For example, it leads to the use of empirical relations to describe dynamic processes that are not fully understood. Also important to mention is the required computational effort for solving partial differential equations. Hence, simpler models are advocated whenever this is appropriate for the task the model has to fulfil. In our research, emphasis is on using models for the understanding of the complete biofilm based unit process and subsequently use them to optimise the process where possible.

The model

For these reasons, a relatively simple mathematical model of the biofilm process was developed (Rauch *et al.*, 1999). The model is an extension to the half-order reaction concept that combines a zero-order kinetic dependency on substrate concentration with diffusion limitation (Harremoës, 1978). The model is solved by means of a two step procedure where (1) the active fraction of the biomass within the biofilm is computed and (2) all conversions within the biofilm are calculated as if the biofilm reactor was an ideally mixed reactor (Figure 1).

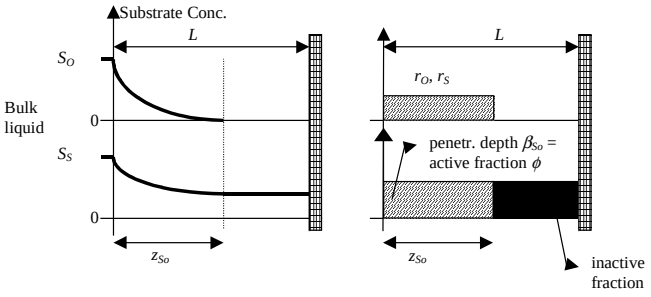

Figure 1. Illustration of a diffusion limited reaction in a system with 2 substrates (S_O being oxygen and S_S being organic matter). S_O is the limiting substrate

Once the active fractions of the biomass have been computed, the biokinetic process description is straightforward. The concepts formulated in the activated sludge model No 1 (Henze *et al.*, 1987) are followed as closely as possible. In Table 1 part of the process matrix of the model is shown. This part describes the aerobic degradation of organic matter.

Table 1. Process matrix for aerobic processes in the biofilm and corresponding effect to the concentration of soluble components in the bulk liquid

	Bulk Liquid				Biofilm			
Process	S_O ML^{-3}	S_S ML^{-3}	S_{ND} ML^{-3}	S_{NH} ML^{-3}	X_{BH} ML^{-3}	X_{BS} ML^{-3}	X_{BI} ML^{-3}	Process rate $ML^{-3}T^{-1}$
aerobic het. growth	$1-1/Y_H$	$-1/Y_H$		$-i_x$	1			$\mu_H.X_{FBH}.\phi_H$
decay heterotrophs					-1	1-fp	fp	$b_H.X_{BH}$
hydrolysis of X_{BS}		1		i_x		-1		$k_h.X_{BS}$
hydrolysis of S_{ND}			-1	1				$k_a.S_{ND}$

Application of the model

This modelling approach was applied to two different biofilm plants. Both were trickling filter systems, however, the first plant was treating mainly domestic wastewater with quite a low loading rate. The second plant was treating a heavily loaded industrial wastewater.

Case study 1

As mentioned before, the first trickling filter system is treating mainly sewage wastewater. The trickling filter has a volume of 1400 m^3 and is filled with a PVC carrier material of the "cross flow"-type. A *COD* removal of 57 % is obtained (influent flow 181 m^3/h, COD 480 mg/l). When the *COD* removal is plotted against the *COD* load to the filter system, an apparent linear dependency may be deduced (Figure 2).

The hydraulic set-up of the plant was verified with a tracer test using LiCl and was implemented in the WEST simulator (Hemmis NV, Kortrijk, Belgium) (Figure 3). The simple biofilm could be simplified. During the operation of the system, no nitrification or denitrification activity could be observed. Consequently, only aerobic heterotrophic activity was modelled (Table 1).

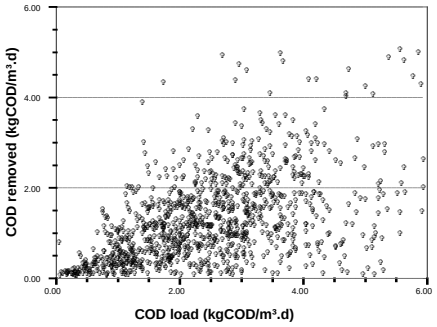

Figure 2. Removal rate of the trickling filter system vs. its loading rate

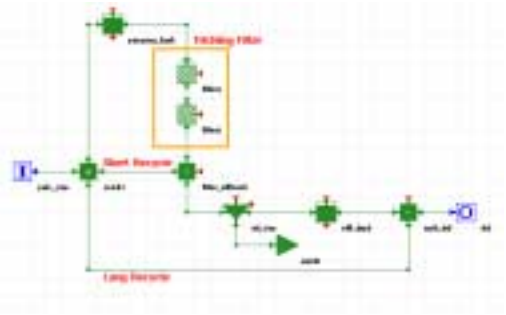

Figure 3. Layout of the trickling filter system in the WEST simulator

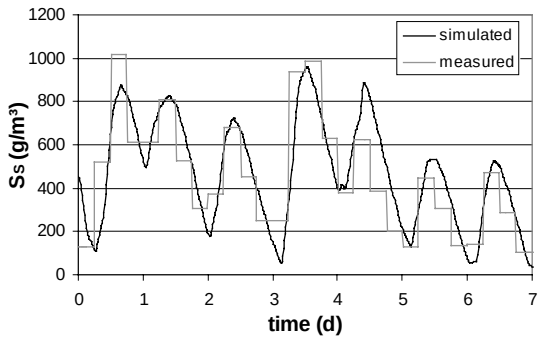

Figure 4. Measured and simulated effluent readily biodegradables (S_S) during the intensive measurement campaign (calibration)

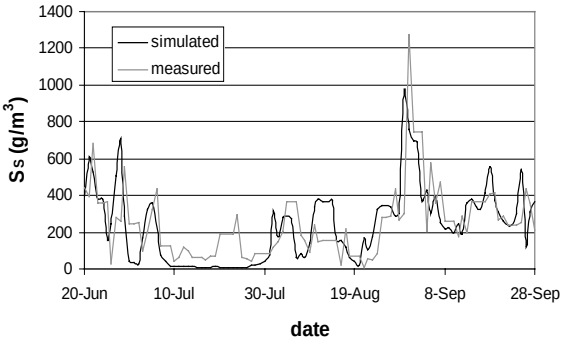

Figure 5. Measured and simulated effluent readily biodegradables (S_S) during the day-to-day operation (validation)

The results of an intensive measurement campaign were used to calibrate the parameters of the model. Extra measurements were used to subdivide the influent measurements into the *COD* and *N* components the model uses. For example, BOD_{28} tests were performed to determine the inert fraction of the *COD*.

Parameters were compiled from various sources and were kept as close as possible to the standard ASM1 parameter set during the calibration (Henze *et al.*, 1987). Only tuning of the K_La (1000 d^{-1}) and the biofilm attachment and detachment coefficients was needed to

calibrate the substrate conversion and the sludge production (Figure 4). The model was validated based on long term measurements during in total about 7 months (Figure 5).

Simulations with the model revealed that the maximum loading rate the trickling filter system can treat is about 2 kg *COD*/m^3.d. In literature, loading rates of 4 to 5 kg *COD*/m^3.d are reported for high rate trickling filter systems. These numbers however require carrier materials with high specific surface areas of more than 200 m^2/m^3. The carrier material used here has a specific surface area of only 100 m^2/m^3. The surface available for biofilm growth limits higher treatment efficiencies. These foundings do not agree with what could be deduced on Figure 2. In this figure a trend for efficiencies surpassing 2 kg *COD*/m^3.d at higher loads was noticed. However, Figure 2 was compiled from point measurements in the influent and the effluent of the filter system. It is very dangerous to compare these measurements since they do not reflect the exact dynamic behaviour of the system.

Case study 2

The plant used for the second case study was an industrial wastewater treatment plant. A characteristic of this WWTP is that the influent concentration of *COD* is extremely high and varies dramatically over time. An on-line measurement of the off-gas O_2 and CO_2 was integrated and used for modelling.

Its biofilm plant consisted of two trickling filters working in parallel. The total reactor volume was 3160 m^3. This volume too is filled with a PVC carrier material of the "cross-flow"-type. The organic load of the plant equals 15000 kg *COD*/d (the flow rate was 110 m^3/h).

The model described above was extended with a model for the description of the carbon dioxide production rate (*CPR*) in the biofilm reactor, partly based on the model developed by Spérandio and Paul (1997). The *CPR* is, however, not directly measurable because the production of inorganic carbon (*IC*) by bacterial conversion takes place in the form of $CO_{2,aq}$. The dynamic equilibria in which CO_2 plays a role result in a distribution of CO_2 over the liquid and the gas phase so that a *CTR* (CO_2 transfer rate), rather than a *CPR*, is measured (Govind *et al.*, 1997):

$$\begin{array}{ccccccc} CTR^{measured} & & CPR^{reality} & & & & \\ \uparrow & & \downarrow & & K_1 & & K_2 \\ CO_2^{(gas)} & \Leftrightarrow & CO_2^{(aq)} & \Leftrightarrow H_2CO_3 & \Leftrightarrow HCO_3^- + H^+ & \Leftrightarrow & CO_3^{2-} + 2H^+ \end{array} \quad (1)$$

In this model, the *IC*-equilibrium is modelled kinetically. For instance, the *pH*-dependent production rate of bicarbonate can be written as:

$$r_{HCO_3^-} = k_1[CO_{2,aq}] - k_{-1}[HCO_3^-][H^+] + k_2[CO_{l,aq}][OH^-] + k_{-2}[HCO_3^-] \quad (3)$$

The mass transfer between gas and liquid phase for carbon dioxide is expressed as:

$$\Phi_{CO_2}^{G\to L} = CTR = K_L a \cdot \left([CO_{2,aq}]^* - [CO_{2,aq}]\right) \cdot V \quad \text{with} \quad [CO_{2,aq}]^* = \frac{p_{CO_2}}{H} \quad (4)$$

where *H* is the Henry's constant for CO_2 ($atm^{-1}M$).

The calibration of the model was more difficult than the in case study 1. The model parameters were adapted to fulfil:

1. The sludge balance: It was chosen to adjust attachment and detachment model coefficients to approximate the suspended solids measurements since good data about the sludge production were not available. To have an extra check on the sludge balance, the removal of nitrogen from the system was monitored.

2. The effluent concentrations: The parameters to which the model is most sensitive in this respect are the specific growth rate μ_{max}, the decay rate b_H and the yield coefficient Y_H. For this case study, lab experiments showed that the well-accepted yield (Henze *et al.*, 1987) of 0.67 is too high and that a value of 0.5 is more appropriate (Petersen, 2000).

3. The off-gas concentrations: The model parameters should be adapted to make the predictions follow the measured off-gas concentrations. Particularly, the knowledge of *IC* in both the liquid and the gas phase can be used to obtain good estimates of the K_La for CO_2 and thus also for O_2. It can be shown that $(K_La)^{CO2} \approx 0.9(K_La)^{O2}$ = 4500 d^{-1} (Spérandio and Paul, 1997).

The calibration results are given in Figure 6 and Figure 7.

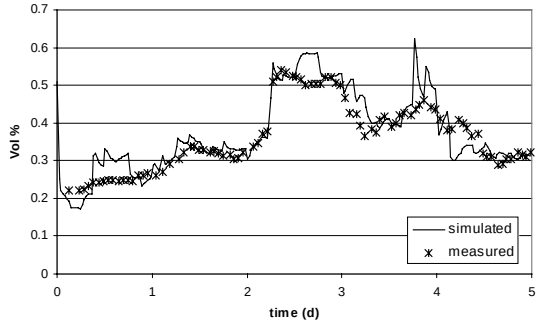

Figure 6. Measured and simulated off-gas CO_2 *concentration*

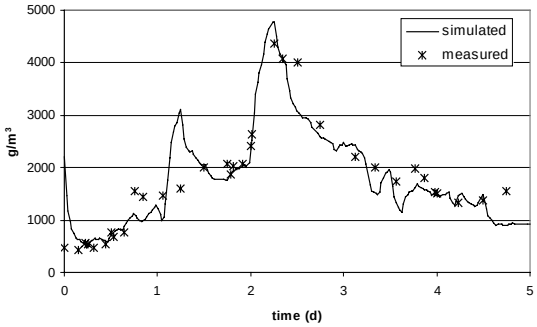

Figure 7. Measured and simulated effluent readily biodegradable substrate (S_S)

Conclusions

A model, based on the simple multispecies biofilm model developed by Rauch *et al.* (1999), was built and calibrated to describe the biodegradation in two trickling filter systems. The calibration was based on the results of intensive measurement campaigns. The limited biodegradation capacity of the filter in the first case study was clearly demonstrated by the model. During the second case study, off-gas analysis was used to monitor the O_2 and CO_2 content of the off-gasses. The model therefore was extended with a section describing the production and transport of CO_2 and inorganic carbon (*IC).*

Acknowledgement

The project was financially supported by the Institute for the Promotion of Innovation by Science and Technology in Flanders (IWT). The first author is a Research Assistant of the Fund for Scientific Research - Flanders (Belgium). The authors would like to acknowledge KELMA bvba (Niel, Belgium) who provided the off-gas measurement equipment.

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