Presentation and evaluation of the zero-dimensional biofilm model 0DBFM

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ABSTRACT

A zero-dimensional biofilm model, i.e. 0DBFM, has been developed for dynamic simulation of moving bed bioreactors (MBBRs). This mini-review aims at presenting and evaluating 0DBFM. 0DBFM is presented in Petersen matrix format and is based on the activated sludge model ASM1, which is an explicit and quite complex model (eight processes, 13 state variables, and 19 parameters) that has found wide application in engineering practice. 0DBFM is thus based on existing knowledge in biological wastewater treatment. The ASM1 approach has been confirmed by respirometry since the resulting respirograms were successfully simulated with ASM1. 0DBFM distinguishes between attached and suspended biomass and incorporates attachment of suspended matter from the bulk liquid onto the biofilm and detachment of biofilm into the bulk liquid. Still, 0DBFM respects the golden rule of modelling, which says that 'models should be as simple as possible and as complex as needed' and resists Occam's razor. The practicability of 0DBFM has been shown on a pilot-scale plant since nine days of wastewater treatment were successfully simulated and effluent quality was dynamically predicted. Finally, 0DBFM can be inspiring and the applicability of 0DBFM to other biofilm systems can be tested.

Key words | biofilm, modelling, Occam's razor, simulation, wastewater, zero-dimensional biofilm model

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INTRODUCTION

The water resource recovery facility (WRRF) of Hesperange in Luxemburg was modernised and upgraded with moving bed bioreactor (MBBR) technology. In this context, a scientific support with emphasis on process modelling and simulation was carried out.

Note that a gap between biofilm research and engineering practice has increased over the past decades in the biofilm modelling community. The reasons for this have been discussed in the literature (Noguera *et al.* 1999; Morgenroth *et al.* 2000a). Considerable research has therefore been dedicated to the topic and an excellent overview of available biofilm models can be found in the *IWA Scientific and Technical Report No. 18* (Eberl *et al.* 2006). However, there is still a need to develop biofilm models that can be used in engineering practice. In particular, there is a need for biofilm models that can predict WRRF effluent quality in response to influent variations. One-dimensional (1D) biofilm models have been mostly used for this purpose since there was a trend from more complex two- and three-dimensional (2D and 3D) models towards 1D models for application in engineering practice (Morgenroth *et al.* 2000b). Although 1D models have been proposed since the 1970s (Wuertz & Falkentoft 2003), calibration protocols for 1D models are still under development (see for example Barry *et al.* 2012 and Rittmann *et al.* 2018) and still need to be established in the engineering community. This illustrates how difficult the application of even relatively simple 1D biofilm models is in engineering practice. After the author of this contribution had a negative experience with a 1D biofilm model, the objective of the research presented here became to develop a biofilm model for engineering practice.

It was observed that the biofilm, which was attached to the carriers in a pilot-scale plant, had a complex three-dimensional structure with cell clusters, pores and channels, not in line with the simple schematic one-dimensional representation of a biofilm but more of an activated sludge matrix. The idea came to model the MBBR with an activated sludge model, i.e. ASM1 (Henze *et al.* 2000). This approach

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resulted in 0DBFM, a zero-dimensional (0D) biofilm model that can dynamically predict effluent quality in response to influent variations and that is presented and evaluated here. A brief account of the methods that were employed is given in order to facilitate understanding of what has been done.

METHODS

The methods regarding wastewater analysis, operation of the pilot-scale plant, and respirometry are described in detail elsewhere (Plattes *et al.* 2006, 2007). A brief account of what has been done is given here. The pilot-scale MBBR was composed of three subsequent compartments. The first and second compartment (2.8 m^3 each) were filled with Kaldnes (K1) carrier elements with a filling degree of 50% and 65% respectively. The third compartment was used as a settling tank. During the first measurement campaign (5 d) the first and the second compartment were both aerated, i.e. nitrification mode. The inflow was 21.4 m^3/d of raw municipal wastewater. During the second measurement campaign (4 d) the first compartment was anoxic, the second compartment was aerated, and nitrates were recycled from the settling tank to the first compartment, i.e. denitrification mode. The inflow was 17.05 m^3/d and the nitrate recycle was 22.25 m^3/d (recycle ratio 1.3). The MBBR had attained stable operation before the measurement campaigns took place. During the first measurement campaign (nitrification mode) 6 h composite samples of influent and effluent were analysed for standard wastewater parameters. During the second measurement campaign (denitrification mode) 4 h composite samples were analysed for the same parameters and respirometric experiments were carried out according to the static gas static liquid principle (Spanjers *et al.* 1998). The respirograms were simulated with the WRRF simulator GPS-X (Hydromantis Inc.) using ASM1 (Henze *et al.* 2000). The resulting kinetic parameters were transferred to the proposed zero-dimensional biofilm model, that was also implemented in GPS-X. The amount of biofilm (biofilm solids) and the amount of suspended solids in the reactor were also measured.

PRESENTATION OF 0DBFM

The mass balances of 0DBFM are analogous to the mass balances in activated sludge models, with the only difference being that biofilm remains in the reactor: the rate of change of dissolved state variables (S_i) with respect to time (t) equals the hydraulic flow (Q) divided by the reactor volume (V) multiplied by the difference between the concentration in the influent ($S_{i,in}$) and the concentration in the effluent ($S_{i,out}$) plus the rate in the zero-dimensional biofilm model (r_{0DBFM}) (Equation (1)). The rate of change of suspended particulates (X_i^S) (Equation (2)) is analogous to Equation (1). The rate of change of attached (biofilm) particulates (X_i^B) is simply given by the rate of change of 0DBFM (r_{0DBFM}), because biofilm does not enter or leave the reactor with the hydraulic flow (Equation (3)).

$$\frac{dS_i}{dt} = \frac{Q}{V}(S_{i,in} - S_{i,out}) + r_{\mathrm{0DBFM}} \quad (1)$$

$$\frac{dX_i^S}{dt} = \frac{Q}{V}(X_{i,in}^S - X_{i,out}^S) + r_{\mathrm{0DBFM}} \quad (2)$$

$$\frac{dX_i^B}{dt} = r_{\mathrm{0DBFM}} \quad (3)$$

0DBFM has been presented in Petersen matrix format and contains 29 processes, 21 state variables and 28 parameters, and is presented here as published in the literature (Plattes *et al.* 2008). The biochemical conversions in 0DBFM are as given in ASM1. They apply to attached and suspended biomass and are a function of the concentration of substrates in the bulk liquid. Diffusional mass transfer limitations manifest by adapted half-saturation indices in the Monod terms of 0DBFM.

Further, 0DBFM has attachment of suspended solids from the bulk liquid onto the biofilm and detachment of biofilm into the bulk liquid. Attachment rate (r_a) and detachment rate (r_d) are formulated according to a detachment rate expression proposed in the literature (Trulear & Characklis 1982). It is assumed that the attachment rate is proportional to the square of the amount of suspended solids (SS) and that the detachment rate is proportional to the square of the amount of biofilm solids (BS), the proportionality factor being the attachment rate constant (k_a) and the detachment rate constant (k_d) respectively (Equations (4) and (5)). Attachment and detachment rates are formulated individually for each particulate state variable in 0DBFM, whilst the values of k_a and k_d are maintained as constant (see Plattes *et al.* 2008 for further explanation).

$$r_a = k_a \cdot (SS)^2 \quad (4)$$

$$r_d = k_d \cdot (BS)^2 \quad (5)$$

The model therefore distinguishes between hydraulic residence time (HRT) and residence time of biofilm on the substratum, which is called the biofilm age (BA). Biofilm age can be estimated using simulation results and Equation (6). Biofilm age can be estimated only, because the detachment rate is not measurable.

$$\mathrm{BA} = \frac{\text{Amount of biofilm}}{\text{Detachment rate}} \tag{6}$$

0DBFM does not incorporate biofilm structure in any form and therefore does not contain any parameter related to biofilm structure (like biofilm thickness).

Kinetic parameters are obtained from respirometry, if available, for model calibration. Otherwise, calibration can be started with default values of ASM1. Further model calibration is achieved using two iterative steps:

Step 1: The attachment and detachment rate constants are adjusted in order to match the biofilm solids in the compartment.

Step 2: The detachment rate constant is further adjusted in order to produce the required biofilm age and nitrification rate using the effluent ammonium and/or nitrate concentration.

Step 2 changes the amount of biofilm (biofilm solids) and the attachment rate needs to be readjusted. Steps 1 and 2 become iterative in the procedure.

Kinetic parameters can be further adjusted using the effluent data. Note that half-saturation indices can be adjusted individually for attached and suspended biomass.

DISCUSSION AND EVALUATION OF 0DBFM

0DBFM is based on ASM1 (Henze *et al.* 2000) and hence the Monod model (Monod 1949). The Monod model gives a functional relation between specific growth rate and substrate concentration in the *bulk*. ASM1 and the Monod model have found wide application in engineering practice so far. 0DBFM is thus based on existing and well-established knowledge in biological wastewater treatment modelling and biochemical engineering.

In activated sludge models (ASMs) the Monod model is implemented to describe the macrokinetic behaviour of activated sludge reactors, not explicitly describing concentration gradients in the activated sludge floc (Plattes 2009). Diffusional mass transport limitations are taken into account implicitly by adapted values of the half-saturation indices in ASM1, which are a function of various processes in activated sludge systems (Arnaldos *et al.* 2015). So far, in biofilm modelling the Monod equation has been used to model intrinsic kinetics of the biofilm, since diffusion is usually described explicitly using Fick's laws of diffusion. In 0DBFM, the Monod model is used to describe the macrokinetic behaviour of biofilm reactors, analogous to the use of the Monod model in state of the art activated sludge models (ASMs). The role that biofilm and floc structure have played in this context has been thoroughly discussed in the literature (Plattes 2009). Essentially, it is stated that biofilm structure has been strongly emphasized in the biofilm modelling community (1D, 2D, 3D), whilst state of the art activated sludge models do not take structure into account, i.e. they are zero-dimensional (0D). The author believes that the application of Fick's laws of diffusion, which crucially link diffusional mass transfer to biofilm structure, has been a driving force for biofilm model development from 1D to 3D, in addition to the fact that biofilms have a complex three dimensional structure (see Wanner 1995 and references in there).

The zero-dimensional ASM1 approach of 0DBFM has been confirmed by respirometry in the laboratory (Plattes *et al.* 2007). The obtained respirograms featured the typical endogenous and exogenous respiration phases and the respirograms could be simulated with ASM1 (Figure 1). The resulting kinetic parameters were transferred to the biofilm model of the pilot-scale MBBR. The fact that the respirograms have the shape of typical respirograms obtained with activated sludge justifies the modelling approach taken by 0DBFM, i.e. modelling a biofilm system with an activated sludge model.

0DBFM has attachment and detachment of biomass, two processes that are in the eyes of the author not measurable, because they are counteractive and simultaneous. In order to avoid unnecessary complexity, attachment and detachment might therefore not be integrated in a biofilm model, although it is recognized that both processes take place in biofilm systems (Hermanowicz 2003), detachment being considered to be a process that is often overlooked (Morgenroth 2003). Indeed, a zero-dimensional biofilm model that ignores both attachment and detachment has been formulated and applied by other researchers (Volcke *et al.* 2008). However, by the author's own experience it was necessary to integrate attachment and detachment in 0DBFM, in order to distinguish between attached and suspended biomass, a prerequisite for the application of the proposed mass balances (Equations (2) and (3)) and the discrimination of hydraulic residence time and biofilm age

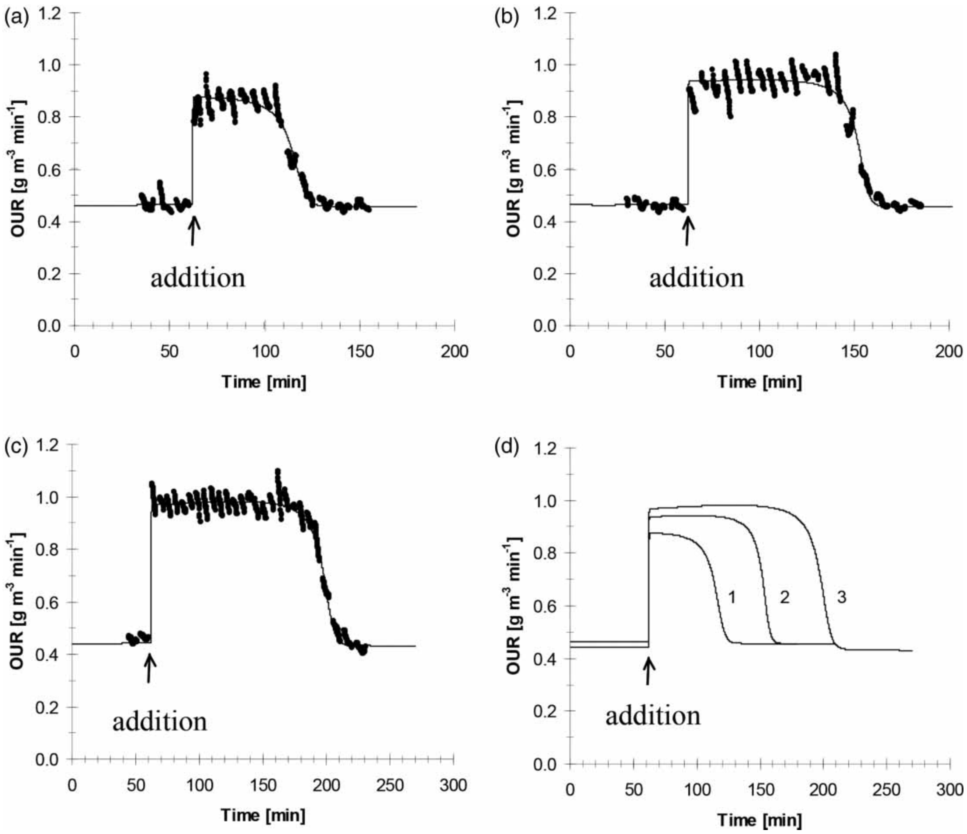

Figure 1 | Measured and simulated respirograms (adapted from Plattes *et al.* 2007) obtained with biofilm samples originating from the pilot-scale MBBR (addition of 5.25 (a), 10.49 (b), and 17.51 mg/l (c) ammonium-N; simulations compared in (d)).

(Equation (6)). A similar approach including attachment and detachment has been taken previously in a pure simulation study to model a continuous stirred tank biofilm reactor (Chen & Chai 2005). Further, the simulation results give at least a quantitative estimation of what the attachment and detachment rate possibly could be, which is interesting since real data regarding these rates are scarce or non-existent. Note that estimation of attachment and detachment rate is also possible with 1D biofilm models.

The proposed calibration procedure is relatively simple because no structure related parameters (like biofilm thickness) need to be calibrated.

The practicability of 0DBFM has been demonstrated on the pilot-scale plant: nine days of wastewater treatment were successfully simulated and the dynamic variations of ammonium and nitrate nitrogen were accurately predicted by 0DBFM (see Figure 2 for a five day simulation result).

Although 0DBFM is quite complex and explicit it respects the golden rule of modelling, which says that ‘models should be as simple as possible and as complex as needed’. Further 0DBFM conforms to the principle of parsimony and resists Occam’s razor in contrast to 1D, 2D and 3D biofilm models.

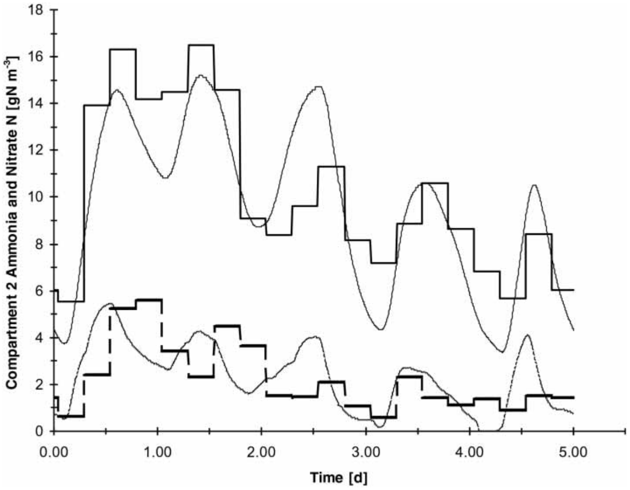

Figure 2 | Simulated (waved) and measured (stepped) ammonium (bottom) and nitrate (top) nitrogen concentration in the effluent of the pilot-scale MBBR operated in nitrification mode (adapted from Plattes *et al.* 2008).

Finally, the zero-dimensional biofilm modelling approach can be inspiring and the applicability to other wastewater treatment systems like fixed bed reactors and granular sludge reactors, for example, could be tested.

CONCLUSIONS

A fundamental problem has been overcome by 0DBFM: modelling biofilm structure. It is therefore believed that 0DBFM can possibly help in reducing the gap that has developed over the past decades between biofilm research and engineering practice in the biofilm modelling community. The predictive power of 0DBFM should be further tested on pilot- and full-scale plants and the simulation results should be compared to 1D models. Long term model performance should be evaluated.

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REFERENCES

Arnaldos, M., Amerlinck, Y., Rehman, U., Maere, T., Van Hoey, S., Naessens, W. & Nopens, I. 2015 From the affinity constant to the half-saturation index: understanding conventional modelling concepts in novel wastewater treatment processes. *Water Research* **70**, 458–470.

Barry, U., Choubert, J. M., Canler, J. P., Héduit, H., Robin, L. & Lessard, P. 2012 A calibration protocol of a one-dimensional moving bed bioreactor (MBBR) dynamic model for nitrogen removal. *Water Science and Technology* **65** (7), 1172–1178.

Chen, L.-M. & Chai, L.-H. 2005 Mathematical model and mechanisms for biofilm wastewater treatment systems. *World Journal of Microbiology & Biotechnology* **21**, 1455–1460.

Eberl, H., Morgenroth, E., Noguera, D. R., Picioreanu, C., Rittmann, B., Van Loosdrecht, M. & Wanner, O. 2006 *Mathematical Modelling of Biofilms* (IWA Task Group on Biofilm Modelling, ed.). Scientific and Technical Report No. 18, IWA Publishing, London, UK.

Henze, M., Gujer, W., Mino, T., Van Loosdrecht, M. C. M. 2000 *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3* (IWA Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment, ed.). Scientific and Technical Report No. 9, IWA Publishing, London, UK.

Hermanowicz, S. W. 2003 Biofilm architecture: interplay of models and experiments. In: *Biofilms in Wastewater Treatment – An Interdisciplinary Approach* (S. Wuertz, P. L. Bishop & P. A. Wilderer, eds). IWA Publishing, London, UK, pp. 32–48.

Monod, J. 1949 The growth of bacterial cultures. *Annual Review of Microbiology* **3**, 371–394.

Morgenroth, E. 2003 Detachment: an often-overlooked phenomenon in biofilm research and modeling. In: *Biofilms in Wastewater Treatment – An Interdisciplinary Approach* (S. Wuertz, P. L. Bishop & P. A. Wilderer, eds). IWA Publishing, London, UK, pp. 264–288.

Morgenroth, E., Van Loosdrecht, M. C. M. & Wanner, O. 2000a Biofilm models for the practitioner. *Water Science and Technology* **41** (4–5), 509–512.

Morgenroth, E., Eberl, H. & Van Loosdrecht, M. C. M. 2000b Evaluating 3-D and 1-D mathematical models for mass transport in heterogeneous biofilms. *Water Science and Technology* **41** (4–5), 347–356.

Noguera, D. R., Okabe, S. & Picioreanu, C. 1999 Biofilm modelling: present status and future directions. *Water Science and Technology* **39** (7), 273–278.

Plattes, M. 2009 The Role of Biofilm and Floc Structure in Biological Wastewater Treatment Modelling. In: *Biochemical Engineering* (F. E. Dumont & J. A. Sacco, eds). Nova Science Publishers, New York, USA, pp. 245–255.

Plattes, M., Henry, E., Schosseler, P. M. & Weidenhaupt, A. 2006 Modelling and dynamic simulation of a moving bed bioreactor for the treatment of municipal wastewater. *Biochemical Engineering Journal* **32**, 61–68.

Plattes, M., Fiorelli, D., Gillé, S., Girard, C., Henry, E., Minette, F., O'Nagy, O. & Schosseler, P. M. 2007 Modelling and dynamic simulation of a moving bed bioreactor using respirometry for the estimation of kinetic parameters. *Biochemical Engineering Journal* **33**, 253–259.

Plattes, M., Henry, E. & Schosseler, P. M. 2008 A zero-dimensional biofilm model for dynamic simulation of moving bed bioreactor systems: model concepts, Peterson matrix, and application to a pilot-scale plant. *Biochemical Engineering Journal* **40**, 392–398.

Rittmann, B. E., Boltz, J. P., Brockmann, D., Daigger, G. T., Morgenroth, E., Sørensen, K. H., Takács, I., van Loosdrecht, M. & Vanrolleghem, P. 2018 A framework for good biofilm reactor modeling practice (GBRMP). *Water Science and Technology* **77** (5), 1149–1164.

Spanjers, H., Vanrolleghem, P. A., Olsson, G. & Dold, P. 1998 *Respirometry in Control of the Activated Sludge Process: Principles*. IAWQ Task Group on Respirometry, Scientific and Technical Report No. 7, IAWQ Publishing, London, UK.

Trulear, M. G. & Characklis, W. G. 1982 Dynamics of biofilm processes. *Journal of the Water Pollution Control Federation* **54**, 1288–1301.

Volcke, E. I. P., Sanchez, O., Steyer, J.-P., Dabert, P. & Bernet, N. 2008 Microbial population dynamics in nitrifying reactors: experimental evidence explained by a simple model including interspecies competition. *Process Biochemistry* **43**, 1398–1406.

Wanner, O. 1995 New experimental findings and biofilm modelling concepts. *Water Science and Technology* **32** (8), 133–140.

Wuertz, S. & Falkentoft, C. M. 2003 Modelling and simulation: Introduction. In: *Biofilms in Wastewater Treatment – An Interdisciplinary Approach* (S. Wuertz, P. L. Bishop & P. A. Wilderer, eds). IWA Publishing, London, UK, pp. 3–7.

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