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Modeling and simulation of membrane bioreactors by incorporating simultaneous storage and growth concept: an especial attention to fouling while modeling the biological process

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Abstract

The major obstacle for membrane bioreactors (MBRs) to become a widely applicable technology is the membrane fouling. Despite the fact that the fouling is inevitable, understanding of the inherent mechanisms and subsequent integrated modeling of the process seems greatly helpful for optimization and control. Several researches have shown the importance of extra-cellular polymeric substances (EPS) their role in explaining the two-step with sudden jump in TMP vs. time. But, the crucial point remains about the prediction of the EPS concentration in the dynamic MBR sludge matrix and the research attention becomes bit more on biological behavior of the sludge matrix in order to have 'an integrated complete dynamic model' describing both filtration and biological behavior simultaneously. Moreover, on account of operational and fundamental difference from conventional wastewater treatment processes, MBRs possess distinct biological dynamics and hence the activated sludge models (ASMs: ASM1, ASM3, etc. [4]) in their original form are not expected to be workable. Therefore, the two-fold idea has been suggested and used for simulation herein are (i) improved version of ASM3 as suggested by Sin et al. [16] seems promising in order to explain the distinct MBR biological process dynamics, and (ii) EPS model which has a strong urge to be used as input to fouling model.

The notion of 'complete model' provides a platform to infuse the researches from two different fields viz. biological process modeling and filtration modeling for MBRs application in a harmonized way and hence provokes interconnected investigations from both the fields.

Keywords: Activated sludge models; ASM3; EPS; Fouling models; MBR modeling; Membrane bioreactors

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1. Introduction

Membrane bioreactor (MBR) technology possess the activated sludge process (ASP) assisted by membrane separation, and considered to be very promising as a modern wastewater treatment technology because of high level of treatment and reduced foot-prints at the same time. However, the major obstacle for MBRs to become a widely applicable technology is the membrane fouling. Despite the fact that the fouling is inevitable, understanding of the inherent mechanisms and subsequent integrated modeling of the process seems greatly helpful for optimization and control.

After the introduction of the critical flux concept (a flux below which no fouling should occur: [2,13]), besides the initial selection of sub-critical flux operation (constant flux filtration), a slow and continuous fouling pattern with sudden jump in transmembrane pressure (TMP) profile has been reported in several researches. Models have been developed, e.g. [13], explaining the fouling behavior in terms of increase in TMP with time during sub-critical flux operation however, any particular fouling species had not been considered. The complexity of fouling mechanism is even instigated by the fact that the MBRs possess distinct biological dynamics i.e. MBR system includes micro-organisms and their unfiltered/retained metabolites [14]. With the progress in researches on the complex nature of MBR sludge matrix, extra-cellular polymeric substances (EPS) are considered to be major fouling species during sub-critical flux operation. Interestingly, a recent research [17] has shown the role of the EPS in explaining the two-step with sudden jump in TMP vs. time. But, the crucial point remains about the prediction of the EPS concentration in the dynamic MBR sludge matrix and the research attention becomes bit more on biological behavior of the sludge matrix in order to have ‘an integrated complete dynamic model’ describing both filtration and biological behavior simultaneously.

The activated sludge models (ASMs: ASM1, ASM3, etc. [4]) in their original form are not expected to be workable for distinct biological process of MBRs. Hence ASMs, along with modifications, have been used for MBR biological process modeling in several researches [10–12]. However, these models do not take into consideration the importance of EPS in explaining and modeling the fouling behavior. On the other hand, filtration modeling researches are unable to incorporate the distinct biological complexity of the MBR sludge matrix. Meaning thereby, in the related researches, harmony is missing among the components used for improving ASMs (tending to explain better the biological process) and those used for fouling behavior modeling.

ASM3 considers the cell mass growth on stored substrates only. And recently, Sin et al. [16] proposed, with scientific soundness, a new approach for modeling simultaneous storage and growth processes, where additional processes have been incorporated into ASM3 stoichiometric matrix. Therefore, the two fold ideas has been suggested and used for simulation herein are (i) improved version of ASM3 as suggested by Sin et al. [16] seems promising in order to explain the distinct MBR biological process dynamics and (ii) EPS model [1] which has a strong urge to be used as input to fouling model after the importance to EPS in explaining two step TMP profile has been observed by Ye et al. [17]. Simulation of the proposed dynamic model has been carried out using AQUASIM (Computer Program for the Identification and Simulation of Aquatic systems).

The research here intends to introduce a framework of ideas with scientific soundness taking into most consideration an applied dynamic modeling. The idea presented here provokes the development of simple EPS prediction model. Idea of infusing such models to MBR biological process model would lead to a complete model for application purpose. The paper here incorporates the recent development in both the fields viz. activated sludge modeling and fouling phenomenon, and tends to propose a comprehensive modeling strategy for MBRs, which is expected to help significantly to MBR process optimization, regardless of the major bottleneck i.e. membrane fouling.

2. The model background and development

2.1. Biological process model

The distinguishable feature of ASM3 [6] is the inclusion of storage phenomenon where the biodegradable substrate has been deemed to be first up-taken and stored by microorganisms (during feast) and used further for biological metabolism (during famine). The concept seems promising in the case of MBRs as the associated biological conditions generally possess high biomass concentration, high SRT and low F/M ratio, and thereby, more chances for microorganisms to face the feast and famine periods. The concept however has been prone to skepticism as the growth on direct substrate uptake was not considered at all. Consequently, the simultaneous storage and growth concept for activated sludge systems proposed by Sin et al. [16] provides a more sound biological process description alternative.

Moreover, a second order model has been proposed by Sin et al. [16] for the description of degradation of the storage products under famine conditions. Noticeably, the degradation of stored materials by microorganisms is the rate-limiting step for the famine conditions; however, there is no common consensus on any one kinetic model. Two widely described kinetic models viz. surface saturation type and first order model have been reasoned to encompass inconsistencies while being considered for full-scale applications. The first one (e.g. as in ASM3) has been shown to cause severe practical identifiability problems due to its structure, resulting in unrealistic parameter estimates [5]; and the later one was developed and applied for experimental conditions and reasoned not to be applicable to full-scale application where the associated storage metabolism is diverse [16].

In order to explain the simultaneous storage and growth, it has been hypothesized that a fraction of substrate flux is diverted to storage and remaining is used for direct cell growth, and that the ratio of storage products to substrate taken up is constant around a certain value.

The kinetic expression describing the degradation of storage products is

$$f\left(\frac{X_{\mathrm{STO}}}{X_{\mathrm{H}}}\right)=\frac{\left(\frac{X_{\mathrm{STO}}}{X_{\mathrm{H}}}\right)^2}{K_2+\left(\frac{X_{\mathrm{STO}}}{X_{\mathrm{H}}}\right)\cdot K_1}$$

where K_1 is the regulation constant of the biomass as function of $X_{\mathrm{STO}}/X_{\mathrm{H}}$ and $K_2 = K_{\mathrm{STO}} * K_1$.

Rate of direct aerobic growth on substrate:

$$\mu_{\mathrm{MAX,S}}\cdot\frac{S_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\cdot\frac{S_{\mathrm{O}}}{K_{\mathrm{O}}+S_{\mathrm{O}}}\cdot\frac{S_{\mathrm{NH}}}{K_{\mathrm{NH}}+S_{\mathrm{NH}}}\cdot\frac{S_{\mathrm{HCO}}}{K_{\mathrm{HCO}}+S_{\mathrm{HCO}}}\cdot X_{\mathrm{H}}$$

Rate of aerobic growth on storage products:

$$\mu_{\mathrm{MAX,STO}}\cdot\frac{S_{\mathrm{O}}}{K_{\mathrm{O}}+S_{\mathrm{O}}}\cdot\frac{S_{\mathrm{NH}}}{K_{\mathrm{NH}}+S_{\mathrm{NH}}}\cdot\frac{S_{\mathrm{HCO}}}{K_{\mathrm{HCO}}+S_{\mathrm{HCO}}}\cdot\frac{\left(\frac{X_{\mathrm{STO}}}{X_{\mathrm{H}}}\right)^2}{K_2+\left(\frac{X_{\mathrm{STO}}}{X_{\mathrm{H}}}\right)\cdot K_1}\cdot\frac{K_{\mathrm{S}}}{K_{\mathrm{S}}+S_{\mathrm{S}}}\cdot X_{\mathrm{H}}$$

where the entire notations used correspond to ASM3 based terminologies [6,16].

For the modification of the ASM3 stoichiometric matrix, above mentioned rate expressions have been included (in following section dealing with simulation) along with corresponding kinetic rate expression for anoxic conditions.

Ahn et al. [1] used the EPS production model for submerged MBR as Leudeking–Piret equation. The mentioned equation is given as: $\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{EPS}) = k_1\mu X + k_2 X$ where k_1, μ and k_2 are biology related parameters and X is the cell-mass concentration. The equation was originally developed for the fermentation of lactic acid in a batch process and does not includes the EPS loss/degradation mechanism. In most cases where the formation and degradation of EPS/SMP is included into activated sludge models as processes and Monod-type expressions are used, the enhancement in the complexity of modified ASMs becomes obvious. It is commented here that, for the successful modeling of the MBR biological process, incorporation of EPS/SMP formation-degradation equations are not necessary and rather they tend to enhance the practical identifiability problem which is considered important issue of ASM calibration process.

Very simple EPS model is being formulated here which provides a connection between fouling model and biological process model.

$$C_{\mathrm{EPS}} = F \cdot X; \quad F = f(h, T, C_{\mathrm{toxic}})$$

where F is factor (termed here as EPS factor) and function of several kinds of biological stress-generating conditions e.g. hydrodynamics (h), temperature (T), concentration/potential of toxic substances (C_{toxic}) and other possible microbial stress-generating environmental conditions; higher the value of F, higher is cell-mass activity. Indeed, it has not yet been possible to formulate the presence of EPS as a function of simple parameters. As well, the proportions of constituents of EPS (mainly carbohydrates and proteins) have been reported to be versatile and to play very diverse role depending upon environmental conditions [8]. Nonetheless, despite all mentioned variability, experiment/pilot observation based EPS data could be starting point. The EPS formulation strategy here, clearly, does not render a mechanistic outlook; however, it provides a framework of idea and provokes a need for in-depth mechanism understanding and subsequent formulations.

2.2. Fouling behavior model

The study by Ye et al. [17], on the fouling behavior modeling using model EPS (sodium alginate), has shown that the combined standard pore blocking and cake filtration model successfully explains the two-step jump in TMP profile during the long term fouling tests. Recent research by Jang et al. [7] comments on the fouling potential of soluble and suspended part of the mixed liquor matrix render differently. However, there is a common consensus among various researches about the role of EPS in the typical two steps TMP jump based fouling phenomenon. The Ognier's model based on local-flux theory could successfully describe the fouling under initial sub-critical flux operation, without any emphasis on EPS as main foulant. Indeed, the model can be extended and generalized by incorporating EPS. Nevertheless, the possibility of fractioned use of EPS, if reasoned more logically sound through future researches, should be studied in detail for the evaluation of the applicability of the model. Hence, the EPS based Ognier's model (as described below) seems promising for the modeling of sub-critical fouling behavior and thereby able to predict the critical condition fouling.

As per Ognier's model:

$$\mathrm{TMP} = \frac{\mathrm{TMP_o}}{1 - ((\alpha \cdot \mathrm{TMP_o} \cdot t^2)/2)}; \quad \alpha = \frac{k' S_{\mathrm{P}} C_{\mathrm{S}}}{\mu R_{\mathrm{P}}}$$

where k' is the combined constant of proportionality; S_{P} is the open pore section, C_{S} is concentration of foulant; μ is the permeate viscosity and R_{P} is the open pore hydraulic resistance. Here C_{S} is to be considered as C_{EPS} (EPS concentration) which is the output of previously explained biological model. Once the parameter α is calibrated

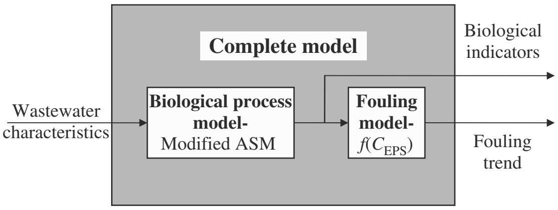

Fig. 1. Schematic representation of the notion of 'complete model'.

for steady state EPS concentration, the model will be expected to show the variation and sudden jump in TMP when the local flux exceeds the critical flux.

2.3. The notion of 'complete model'

The 'complete model' aims at an intelligent coupling of MBR biological process model and fouling behavior model. As depicted schematically in Fig. 1, the fouling model inputs are the outputs of biological process model. And, the outputs of the 'complete model' are outputs from both sub-models.

Remarkably, MBR biological process understanding and subsequent model development is the key step towards the 'complete model'. Thereby, the notion here urges on the recognition of key foulant(s) of biological origin, associated fouling mechanism(s) and potential, environmental dependencies and dynamics.

3. Simulation strategy

Process rate equations and along with corresponding stoichiometric coefficients as per modified ASM3 have been coded into AQUASIM (Computer Program for the Identification and Simulation of Aquatic systems) simulation base [15]. The program consists of four windows viz. variables, processes, compartments and links. The variables of the modified ASM3 (described in Section 2.1) have here been categorized into appropriate categories; three completely mixed compartments have been selected viz. denitrification, nitrification and membrane tank. None of the biological processes have been selected active in the membrane tank. Table 1 lists the wastewater characteristics and other details of the

Table 1
Inputs used in the simulation process

Influent wastewater characteristics[a]		Reactors and conditions	Bio-kinetic parameters
COD, mg/L	500	Denitrification tank	
S_{NH}, mg N/L	30	volume = 5.4 m^3	
S_{NO}, mg N/L	1	Nitrification tank	All the MBR specific bio-kinetic
S_{ALK}, mM HCO$_3$/L	1	volume = 11.4 m^3	parameters have been selected with
S_S, mg COD/L	100	Membrane tank	the help of Judd, [9]; and from
S_I, mg COD/L	25	volume = 1.4 m^3	Sin et al., [16].
X_H, mg COD/L	75	Inflow = 26 m^3	EPS factor value = 50 mg/g X,
X_I, mg COD/L	50	Recirculation ratio = 6	has been selected (pilot study by
X_A, mg COD/L	0	O$_2$ in nitrification	Germain et al., [3]).
X_S, mg COD/L	250	tank = 2 mg/L	
X_{TS}, mg TSS/L	250	SRT = 20 d	

[a] The notations correspond to ASM3 terminology [6].

simulated system. The filtration system (membrane tank) has been shown connected to the nitrification tank through defined links and recirculation has been defined back to denitrification tank which also receives the influent wastewater.

As discussed in introduction, the MBR biology is distinct, the Monod-based biological constant have adopted from Judd [9], where they are extensively summarized and enlisted corresponding to varying conditions from several MBR pilot studies.

4. Simulation results and discussion

Simulation result for the treated effluent (Fig. 2) shows that the total effluent COD remains around 30 mg/L and that the biodegradable portions is almost negligible (less than 5 mg/L) presenting very typical large pilot scale MBR treating municipal wastewater. As well, since input wastewater characteristics used in simulation kept similar to those of municipal wastewater, treated effluent characteristics in terms of nutrient (nitrogen) also seem satisfactory (ammonical nitrogen < 1 mg N/L). Fig. 3 shows the variation is biomass fractions and presents a satisfactory trend. Simulation result depicted in Fig. 4 shows that, by using a typical EPS factor (*F*) corresponding to particular MBR sludge type (high sludge age, low activity, hence low value of *F*), a EPS variation trend can be obtained depending upon variations in *X* (mixed liquor concentration). The EPS prediction can hence be used, as per the notion of 'complete modeling' for the calibration of α parameter of the Ognier's model. Thereby, for a give membrane characteristics and flux flow (constant flux operation), the variation in TMP can be modeled and subsequently, the critical condition correspond to sudden TMP-jump can be predicted.

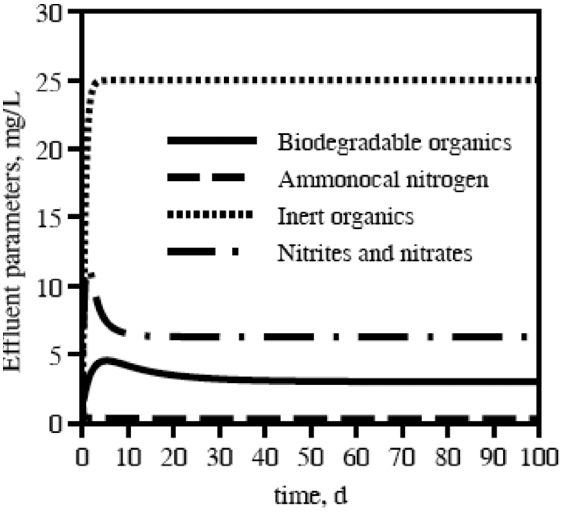

Fig. 2. Simulations results for the properties of treated effluent from MBR.

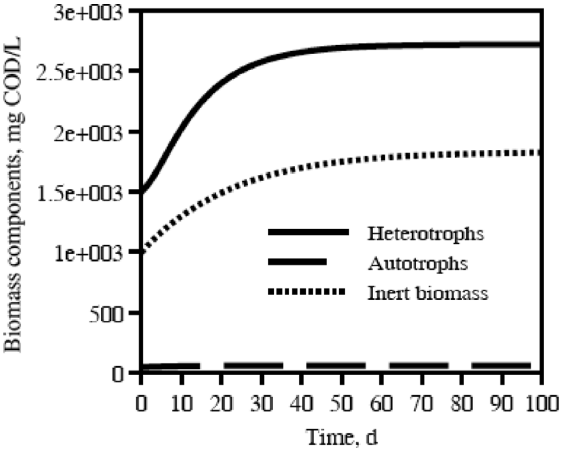

Fig. 3. Simulation of the biological dynamics in MBR.

Of course, simulation results here are representing an overall trend rather than absolute representative values, because of simplification and assumptions while implementing the kinetic parameters into the model simulation. The results however seem satisfactory, showing compatibility with general MBR treatment process and intend to indicate a road-map of simulation of MBR system including simultaneous growth and storage concept after rigorous calibration of modified ASM3.

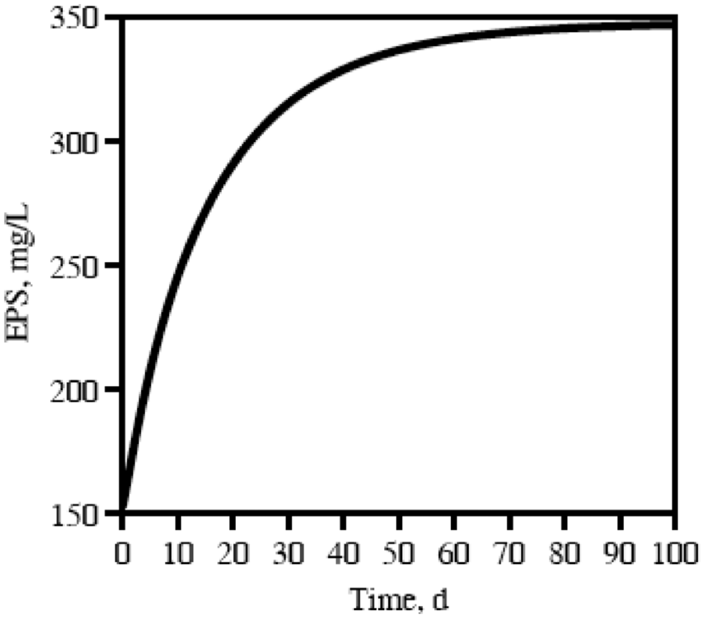

Fig. 4. Simulation of variation in EPS through the course of time.

5. Conclusions

The main conclusions are

- The notion of ‘complete model’ provides a platform to infuse the researches from two different fields viz. biological process modeling and filtration modeling for MBRs application in a harmonized way and hence provokes interconnected investigations from both the fields.
- The modified ASM3 by incorporating simultaneous growth and storage phenomenon seems promising for MBR biological process; it describes treatment performance successfully. The concept aims at better understanding to the microbiological mechanism and helps in avoiding inclusion of bulk parameters like EPS or SMP for describing the biological dynamics.
- An alternative approach can be adopted rather than incorporating EPS formation and degradation process kinetic equations into ASMs in order to simplify the calibration efforts.

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