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ScienceDirect

Procedia Engineering 119 (2015) 1318 – 1327

Procedia Engineering

www.elsevier.com/locate/procedia

13th Computer Control for Water Industry Conference, CCWI 2015

ASM1-based activated sludge model with biopolymer kinetics for integrated simulation of membrane bioreactors for wastewater treatment

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Abstract

This paper presents an activated sludge model suitable for modelling membrane bioreactors (MBRs) for wastewater treatment. The model, later referred to as combined EPS and SMP production ASM1-based model (CES-ASM1), extends Activated Sludge Model No. 1 (ASM1) with biokinetics of two types of bacterial biopolymers: soluble microbial products (SMP) and extracellular polymeric substances (EPS). The biopolymer kinetics in CES-ASM1 are, in their majority, borrowed from Laspidou and Rittmann[1] although, as shall be explained in the article, with one conceptual correction a kinetic pathway of biomass associated products (BAP). CES-ASM1 was calibrated on published experimental results from batch and continuous flow laboratory and pilot plant experiments and proved to be in good agreement with measurements. Standard set of parameters was then proposed as a combination of empirically identified and literature values. The model was then used to predict SMP and EPS production in an activated sludge system under various operating conditions.

Peer-review under responsibility of the Scientific Committee of CCWI 2015

Keywords: activated sludge model, MBR, identification, SMP, EPS

1. Introduction

The first major component of a MBR model is a model of its activated sludge reactor. Although several scientists proved that it was possible to predict some behaviour of a MBR system using one of the standard IAWQ activated sludge models (ASMs) combined with a membrane filtration model, e.g. [2], such models are unable to calculate two important quantities characteristic of a MBR, namely concentrations of soluble microbial products (SMP) and extracellular polymeric substances (EPS). These two groups of organic substances are produced as by-products of microbial activity and are found to accelerate membrane fouling, i.e. progressive reduction of membrane's permeability. These substances are also entirely (EPS) or partially (SMP) retained in the system by the membrane. Many researchers, e.g. [3,4] found that SMP are adsorbed inside membrane pores leading to a reduction of pore diameters and thus to an increase of the membrane's total hydraulic resistance. Although EPS cannot enter the membrane pores alike SMP, EPS have been observed to bridge gaps between individual flocs within cake structure thus increasing the

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Peer-review under responsibility of the Scientific Committee of CCWI 2015
doi:10.1016/j.proeng.2015.08.958

cake's specific cake resistance (SCR) and ultimately causing higher total membrane resistance and hence leading to higher trans-membrane pressures (TMPs).

Nomenclature

f_{BAP}	fraction of S_{BAP} produced during biomass decay (gCOD gCOD^{-1})
$f_{EPS,da}$	fraction of X_{EPS} produced during autotrophic biomass decay (gCOD gCOD^{-1})
$f_{EPS,dh}$	fraction of X_{EPS} produced during heterotrophic biomass decay (gCOD gCOD^{-1})
$f_{EPS,a}$	fraction of X_{EPS} produced during autotrophic biomass growth (gCOD gCOD^{-1})
$f_{EPS,h}$	fraction of X_{EPS} produced during heterotrophic biomass growth (gCOD gCOD^{-1})
f_P	fraction of biomass leading to particulate products (gCOD gCOD^{-1})
f_S	fraction of S_S produced during X_{EPS} hydrolysis (gCOD gCOD^{-1})
f_{T1}, f_{T2}	temperature dependency coefficients (–)
i_{XB}	nitrogen (N) content of biomass, X_H, X_A (gN gCOD^{-1})
i_{XBAP}	nitrogen (N) content of S_{BAP} (gN gCOD^{-1})
i_{XEPS}	nitrogen (N) content of X_{EPS} (gN gCOD^{-1})
i_{XP}	nitrogen (N) content of products of biomass decay, X_P (gN gCOD^{-1})
$k_{h,EPS,20}$	maximum X_{EPS} hydrolysis rate at 20°C (d^{-1})
K_{ALKH}	half-saturation constant for S_{ALK} in heterotrophic growth (moleHCO_3^- m^{-3})
K_{BAP}	half-saturation constant for S_{BAP} (gCOD m^{-3})
K_{NO}	half-saturation constant for S_{NO} (gN m^{-3})
K_{OH}	half-saturation constant for S_O in heterotrophic growth (gCOD m^{-3})
K_{UAP}	half-saturation constant for S_{UAP} (gCOD m^{-3})
S_{BAP}	concentration of biomass associated products (BAP) (gCOD m^{-3})
S_S	concentration of readily biodegradable substrates (gCOD m^{-3})
S_{UAP}	concentration of utilisation associated products (UAP) (gCOD m^{-3})
X_A	concentration of autotrophic biomass (gCOD m^{-3})
X_{EPS}	concentration of extracellular polymeric substances (EPS) (gCOD m^{-3})
X_H	concentration of heterotrophic biomass (gCOD m^{-3})
X_{MLSS}	concentration of mixed liquor suspended solids (MLSS) (g m^{-3})
T_l	liquid temperature (°C)
Y_A	yield coefficient for autotrophic growth (gCOD gCOD^{-1})
Y_H	yield coefficient for heterotrophic growth on S_S (gCOD gCOD^{-1})
Y_{SMP}	yield coefficient for heterotrophic growth on S_{UAP} and S_{BAP} (gCOD gCOD^{-1})
γ_A	fraction of S_{UAP} produced during autotrophic growth (gCOD gCOD^{-1})
γ_H	fraction of S_{UAP} produced during heterotrophic growth (gCOD gCOD^{-1})
$\mu_{BAP,20}$	maximum specific heterotrophic growth rate on S_{BAP} at 20°C (d^{-1})
$\mu_{UAP,20}$	maximum specific heterotrophic growth rate on S_{UAP} at 20°C (d^{-1})

In order to link membrane fouling to bulk liquid SMP and EPS concentrations, the activated sludge model implemented in the integrated MBR model needs to be able to predict formation and degradation kinetics of these two main biofoulants. This task can be accomplished through development of a brand-new biological model or through extension of the existing one, the latter being a preferred option, as the new model can then be benchmarked against a well-established activated sludge model such as Activated Sludge Model No. 1 (ASM1), Activated Sludge Model No. 2d (ASM2d), or Activated Sludge Model No. 3 (ASM3). The new outputs of this extended biological model, i.e. mixed liquor SMP and EPS concentrations can then be used as arguments in the equations of membrane fouling thus linking the biological model to the membrane fouling model. In order to develop an activated sludge model with SMP and EPS concentrations as additional state variables we took the International Association on Water Quality (IAWQ) Activated Sludge Model No. 1 (ASM1) and extended it with SMP and EPS kinetics proposed by Laspidou and Rittmann in their unified theory for extracellular polymeric substances, soluble microbial products, and active and inert biomass [1].

Although a number of already developed ASM models extended with biopolymer kinetics can be found in the scientific literature, e.g. Lu et al.[5],Oliveira-Esquerre et al.[6],Ahn et al.[7],Ni et al.[8],Jiang et al.[9], these models, as explained in detail in Janus[10], were found to be either conceptually flawed or unable to fulfil the main objective of this paper, i.e. development of a full ASM model with SMP and EPS kinetics for integration with a membrane fouling model. The model of Lu et al.[5] lacked mass balance closure while the model of Oliveira-Esquerre et al.[6] had strong interconnections between biopolymer kinetics and main ASM3 process equations thus creating difficulties, if not making it impossible, to calibrate biopolymer kinetics without sacrificing the prediction quality of other state variables such as, e.g. ammoniacal-N or nitrate concentrations. The model of Ahn et al.[7] was insufficiently described in the original publication and therefore impossible to recreate. The model of Ni et al.[8] could not be considered as a full ASM model as it was mainly focused on the description of biopolymer kinetics and lacked description of some relevant processes such as nitrification and denitrification. Most of the above models were additionally only able to predict SMP concentrations while lacking the description of EPS kinetics [5,6,9].

Since a candidate for a biological model for an MBR reactor could not be selected from already published models, we have developed a new model which, in the opinion of the Authors fixes the shortcomings of the above mentioned models and provides a description of both types of biopolymers, i.e. SMP as well as EPS. This model is described in more detail in the next section. However, before we move to the description of our activated sludge model it is important to mention that CES-ASM1 implements the same biopolymer kinetics as an earlier published combined EPS and SMP production ASM3-based model (CES-ASM3) of Janus and Ulanicki[11]. However the Authors felt the need to create an ASM-based model in addition to an already created ASM3-based model because ASM1 is used as a biological model in the COST simulation benchmark [12] as well as the MBR benchmark of Maere et al.[13] and thus the simulation results from CES-ASM1 can be easily compared with the results from both benchmark models. A development of a new MBR benchmark model is currently underway.

2. Model description

As already mentioned in the abstract, CES-ASM1 expands the ASM1 model of Henze et al.[14] with the unified model of production and degradation of SMP and EPS by Laspidou and Rittmann[1] whilst adding a conceptual correction to Laspidou and Rittmann's BAP formation kinetics. While Laspidou and Rittmann assume that all BAP in the system originate from EPS hydrolysis researchers such as Aquino and Stuckey[15] postulated that BAP are additionally produced during bacterial cell decay. In fact, BAP had already been defined earlier by Lu et al.[5] as the SMP fraction strictly originating from biomass decay. The lack of direct active cell decay-related SMP production in Laspidou and Rittmann[1] was found by Menniti and Morgenroth[16] to be the main cause of discrepancies between the predicted SMP concentrations and the measurements. Therefore CES-ASM1 fixes this shortcoming by enabling BAP to be produced in biomass decay. The resulting metabolic SMP and EPS kinetic pathways in CES-ASM1 are visualised in Fig. 1.

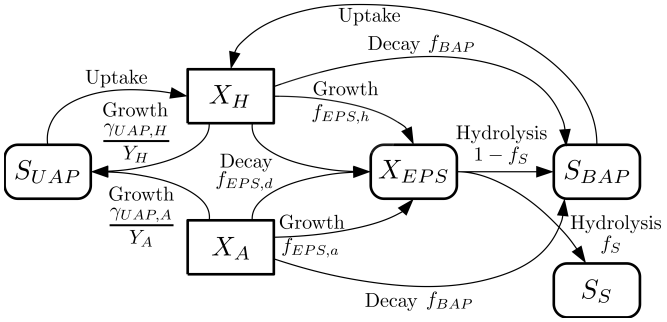


Fig. 1: EPS and SMP formation and utilisation pathways in the biological model.

Similarly to other published biopolymer models SMP are subdivided into utilisation associated products (UAP) and biomass associated products (BAP), whilst EPS are described with just one variable. Production of EPS obeys the Leudeking-Piret equation [17] in which the rate of EPS production is proportional to biomass growth rate as well as the biomass decay rate whilst being in negative proportion with EPS concentration (X_{EPS}). Production of UAP is associated with biomass growth whereas BAP originate from biomass decay and hydrolysis/dissolution of EPS. UAP as well as BAP are taken up by heterotrophic biomass (X_H) for growth and respiration. Both SMP fractions are biodegradable but the degradation kinetics of BAP are assumed to be slower from the degradation kinetics of UAP and readily biodegradable substrates (S_S), after a suggestion of Cho et al.[18].

Before we move to an explanation of the biopolymer process rate equations it is important to note that the CES-ASM1's base model ASM1 has often been criticised for over-predicting denitrification rates in pre-denitrification systems. Such behaviour is a direct consequence of the adopted death-regeneration model in which readily biodegradable substrates (S_S) are cyclically generated as a by-product of biomass decay and provide additional source of carbon for denitrification. The unwanted effects of such model behaviour become significant in long sludge retention time (SRT) systems such as MBRs in which the share of cell maintenance and decay in overall process dynamics is high. However, as described in Janus[10], addition of biopolymer kinetics to ASM1 leads to lower production of readily biodegradable substrates (S_S) as they are substituted as direct products of biomass decay by X_{EPS} and S_{BAP}. Thus the known problem of an overestimation of denitrification rates in ASM1 is, at least partially, eliminated in CES-ASM1.

Process rate equations for SMP and EPS kinetics in CES-ASM1 are listed in Table 1. The remaining kinetic equations have the same form as the original ASM1 equations presented in Henze et al.[19] and are hence omitted. The Petersen matrix for CES-ASM1 is shown in Table 2. The values of stoichiometric and kinetic parameters featured in Table 1 and Table 2 are provided in Table 3. Those parameters which are not listed in Table 3 are assigned the same values as in the original ASM1 model publication of Henze et al.[14]. The unknown stoichiometric parameters in the Petersen matrix denoted with x and y need to be calculated from mass and charge conservation equations. They can also be found in Janus[10, Appendix 1].

Table 1: Process rate expressions for the SMP and EPS kinetics in the biological model.

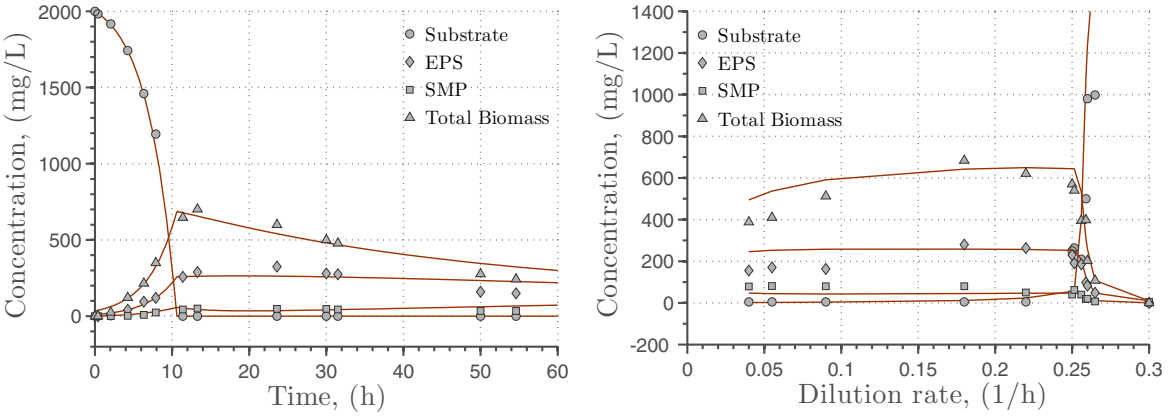
	Process	Process rate equation
$p_{2,b}$	Aerobic growth on S_{BAP}	$f_{T1}\ \mu_{BAP,20}\ \frac{S_{BAP}}{K_{BAP}+S_{BAP}}\ \frac{S_O}{K_{OH}+S_O}\ \frac{S_{ALK}}{K_{ALKH}+S_{ALK}}\ X_H$
$p_{2,c}$	Aerobic growth on S_{UAP}	$f_{T1}\ \mu_{UAP,20}\ \frac{S_{UAP}}{K_{UAP}+S_{UAP}}\ \frac{S_O}{K_{OH}+S_O}\ \frac{S_{ALK}}{K_{ALKH}+S_{ALK}}\ X_H$
$p_{3,b}$	Anoxic growth on S_{BAP}	$f_{T1}\ \mu_{BAP,20}\ \mu_G\ \frac{S_{BAP}}{K_{BAP}+S_{BAP}}\ \frac{K_{OH}}{K_{OH}+S_O}\ \frac{S_{NO}}{K_{NO}+S_{NO}}\ \frac{S_{ALK}}{K_{ALKH}+S_{ALK}}\ X_H$
$p_{3,c}$	Anoxic growth on S_{UAP}	$f_{T1}\ \mu_{UAP,20}\ \mu_G\ \frac{S_{UAP}}{K_{UAP}+S_{UAP}}\ \frac{K_{OH}}{K_{OH}+S_O}\ \frac{S_{NO}}{K_{NO}+S_{NO}}\ \frac{S_{ALK}}{K_{ALKH}+S_{ALK}}\ X_H$
p_7	Hydrolysis of X_{EPS}	$f_{T2}\ k_{h,EPS,20}\ X_{EPS}$

$f_{T1} = e^{-0.069\,(20-T_l)}$

$f_{T2} = e^{-0.11\,(20-T_l)}$

3. Model calibration

The selected kinetic and stoichiometric model parameters were identified on two sets of measurements from two different experiments. The first set of data was obtained from the experiment of Hsieh et al.[20] who investigated SMP and EPS production in a pure bacterial culture of *Pseudomonas atlantica* cultivated in a glucose medium in a batch as well as a continuous flow lab-scale bioreactor. The second set of data was taken from Yigit et al.[21] who measured bulk liquid SMP and EPS concentrations in a submerged MBR pilot plant fed with raw domestic sewage under five different mixed liquor suspended solids (MLSS) setpoints. Whilst the first set of data allowed us to identify the SMP and EPS kinetics, the obtained parameters are characteristic of a single bacterial culture which is likely to have different properties from a typical mixed bacterial population of activated sludge. The second experiment, although did not provide the information necessary for the identification of model dynamics, nevertheless allowed to test the model on the data from an activated sludge system fed with real wastewater. The parameter values obtained from both experiments were then combined with the findings of various researchers in order to derive a set of initial parameter choices for simulation of MBR systems. The model was calibrated after a sensitivity study which revealed the subset of most sensitive parameters with regards to each measured output variable. These most-sensitive parameters were subsequently identified whilst the less sensitive ones were given values from literature. For more information about the experimental and calibration procedures the reader is referred to Janus and Ulanicki[11] and Janus[10] where this information is provided in detail. The identified parameter values are provided in Table 3.



(a) (b)

Fig. 2: Results of CES-ASM1 calibration on batch reactor data (a) and continuous flow reactor data (b) from Hsieh et al.[20,22].

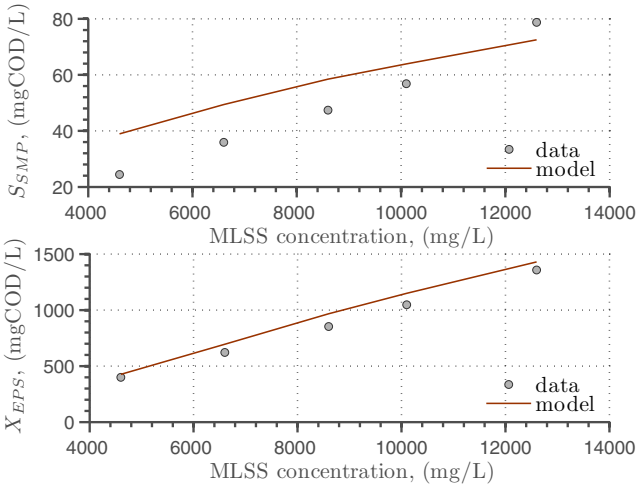


Fig. 3: Results of CES-ASM1 calibration on the experimental data by Yigit et al.[21]

Whilst the first calibration study was based on the measurements from a pure heterotrophic bacterial culture, kinetic and stoichiometric parameters for the autotrophic biomass could not and have not been estimated. It was then assumed that the unidentified SMP and EPS kinetic and stoichiometric parameters for the autotrophic biomass are equal to the corresponding ones for the heterotrophic biomass. Although this is very likely not be true, the relative error this assumption may cause on mixed liquor EPS an SMP concentrations is very small as the autotrophic mass fraction in the activated sludge is roughly only 2% to 5%. Results of both calibration studies are shown in Fig. 2 and Fig. 3 respectively.

Table 2: Stoichiometric (Petersen) and composition matrix for the biological model, *j*: process, *i*: component.

	Model components *i*	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
j	Processes	S_I	S_S	X_I	X_S	X_H	X_{EPS}	S_{UAP}	S_{BAP}	X_A	X_P	S_O	S_{NO}	S_{N_2}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}
	Heterotrophic organisms																	
p_1	Ammonification														1	−1		$\frac{1}{14}$
p_{2a}	Aer. growth on S_S		$-\frac{1}{Y_H}$			$1-f_{EPS,h}$	$f_{EPS,h}$	$\frac{\gamma_H}{Y_H}$				x_{2a}			y_{2a}			$-\frac{i_{XB}}{14}$
p_{2b}	Aer. growth on S_{BAP}					$1-f_{EPS,h}$	$f_{EPS,h}$		$-\frac{1}{Y_{SMP}}$			x_{2b}			y_{2b}			$-\frac{i_{XB}}{14}$
p_{2c}	Aer. growth on S_{UAP}					$1-f_{EPS,h}$	$f_{EPS,h}$	$-\frac{1}{Y_{SMP}}$				x_{2c}			y_{2c}			$-\frac{i_{XB}}{14}$
p_{3a}	Anox. growth on S_S		$-\frac{1}{Y_H}$			$1-f_{EPS,h}$	$f_{EPS,h}$	$\frac{\gamma_H}{Y_H}$					x_{3a}	$-x_{3a}$	y_{3a}			$\frac{1-Y_H}{40\,Y_H}-\frac{i_{XB}}{14}$
p_{3b}	Anox. growth on S_{BAP}					$1-f_{EPS,h}$	$f_{EPS,h}$		$-\frac{1}{Y_{SMP}}$				x_{3b}	$-x_{3b}$	y_{3b}			$\frac{1-Y_H}{40\,Y_H}-\frac{i_{XB}}{14}$
p_{3c}	Anox. growth on S_{UAP}					$1-f_{EPS,h}$	$f_{EPS,h}$	$-\frac{1}{Y_{SMP}}$					x_{3c}	$-x_{3c}$	y_{3c}			$\frac{1-Y_H}{40\,Y_H}-\frac{i_{XB}}{14}$
p_4	Decay of heterotrophs				$1-f_P-f_{EPS,dh}-f_{BAP}$	−1	$f_{EPS.dh}$		f_{BAP}		f_P						$i_{XP}-f_P\,i_{XP}$	
p_5	Hydrolysis of org. compounds		1		−1													
p_6	Hydrolysis of org. N															1	−1	
p_7	Hydrolysis of X_{EPS}		f_S				−1		$1-f_S$							$i_{XEPS}-i_{XBAP}\,(1-f_S)$		
	Autotrophic organisms																	
p_8	Aerobic growth of autotrophs						$f_{EPS,a}$	$\frac{\gamma_A}{Y_A}$		$1-f_{EPS,a}$		$-\frac{\frac{64}{14}-Y_A}{Y_A}$	$\frac{1}{Y_A}$		$-i_{XB}-\frac{1}{Y_A}$			$-\frac{i_{XB}}{14}-\frac{1}{7\,Y_A}$
p_9	Decay of autotrophs				$1-f_P-f_{EPS,da}-f_{BAP}$		$f_{EPS,da}$		f_{BAP}	−1	f_P						$i_{XP}-f_P\,i_{XP}$	
	Composition matrix																	
1	ThOD (g ThOD)	1	1	1	1	1	1	1	1	1	1	-1	$-\frac{64}{14}$	$-\frac{24}{14}$				
2	Nitrogen (g N)					i_{XB}	i_{XEPS}		i_{XBAP}	i_{XB}	i_{XP}		1	1	1	1	1	
3	Ionic charge (Mole$^+$)												$-\frac{1}{14}$		$\frac{1}{14}$			-1

This model assumes that ThOD is identical to the measured chemical oxygen demand (COD). 1 gS_O = -1 gThOD, 1 gS_{NH} = 0 gThOD, 1gS_{NO} = -64/14 gThOD, 1 gS_{N_2} = -24/14 gThOD.

Table 3: Kinetic and stoichiometric parameters for SMP and EPS kinetics of the CES-ASM1 model identified in two calibration studies and reported in literature.

			Calibration 1		Calibration 2				
Parameter	Symbol	Unit	Value	Method	Value	Method	Data set for simulations	Reported values/range	References
ASM1 parameters									
Max. spec. heterotrophic growth rate	$\mu_{H,20}$	d^{-1}	9.35	Fitted	6	Default	6	Default	Henze et al.19
Max. spec. autotrophic growth rate	$\mu_{A,20}$	d^{-1}	0	Assumed	0.8	Default	0.8	Default	Henze et al.19
Yield coefficient for heterotrophic biomass	Y_H	gCOD $gCOD^{-1}$	0.34	Literature *	$0.67/(1+\gamma_H)$	Literature	$0.67/(1+\gamma_H)$	Default	Henze et al.19
Half sat. coeff. for S_S in het. growth	K_S	gCOD m^{-3}	5	*****	20	Default	20	Default	Henze et al.19
CES-ASM1 kinetic parameters									
Max. spec. het. growth rate on S_{UAP}	$\mu_{UAP,20}$	d^{-1}	0.57	Fitted	0***	Assumed	0.45	0.45-0.50	Lu et al.5,Laspidou and Rittmann23
Max. spec. het. growth rate on S_{BAP}	$\mu_{BAP,20}$	d^{-1}	0.135	Fitted	0.0***	Assumed	0.05		
Maximum X_{EPS} hydrolysis rate	$k_{h,EPS,20}$	d^{-1}	0.14	Fitted	0.055	Fitted	0.17	0.03 (anaerobic) - 0.17	Laspidou and Rittmann23, Aquino and Stuckey24
CES-ASM1 stoichiometric parameters									
Fraction of S_{UAP} produced during heterotrophic growth	γ_H	gCOD $gCOD^{-1}$	$0.096\,Y_H$	Fitted	0.092	Fitted	0.092	0.017-0.096	Jiang et al.9,Laspidou and Rittmann23
Fraction of S_{UAP} produced during autotrophic growth	γ_A	gCOD $gCOD^{-1}$	$0.096\,Y_A$	Assumed	0**	Assumed	0 **		
Half saturation constant for S_{BAP}	K_{BAP}	gCOD m^{-3}	85	Literature	85	Literature	85	30-85-500 (anaerobic)	Lu et al.5,Aquino and Stuckey24,Noguera et al.25
Half saturation constant for S_{UAP}	K_{UAP}	gCOD m^{-3}	100	Literature	100	Literature	100	30-100-500 (anaerobic)	Lu et al.5,Aquino and Stuckey24,Noguera et al.25
Yield coefficient for het. growth on SMP	Y_{SMP}	gCOD $gCOD^{-1}$	0.45	Literature	0.45	Literature	0.45		Laspidou and Rittmann23
Fraction of S_{BAP} produced from biomass decay	f_{BAP}	gCOD $gCOD^{-1}$	0.068	Fitted	0.017	Fitted	0.0215	0.0215	Jiang et al.9
Fraction of X_{EPS} produced during X_H cell growth	$f_{EPS,h}$	gCOD $gCOD^{-1}$	0.35	Fitted	0	Assumed	0.18	0.03 (anaerobic) - 0.18	Laspidou and Rittmann23, Aquino and Stuckey24
Fraction of X_{EPS} produced during X_A cell growth	$f_{EPS,a}$	gCOD $gCOD^{-1}$	0.35	Assumed	0	Assumed	0**		
Fraction of X_{EPS} produced from X_H decay	$f_{EPS,dh}$	gCOD $g^{-1}\,X_H$	0.05	Fitted	0.045	Fitted	0.045		
Fraction of X_{EPS} produced from X_A decay	$f_{EPS,da}$	gCOD $g^{-1}\,X_A$	0.05	Assumed	0**	Assumed	0**		
Fraction of S_S produced from X_{EPS} hydrolysis	f_S	gCOD $gCOD^{-1}$	0.4	Fitted	0.4	Assumed	0.4		
N content of S_{BAP}	i_{XBAP}	gN $gCOD^{-1}$	0.07	Literature	0.07	Literature	0.07	0.07	Jiang et al.9
N content of X_{EPS}	i_{XEPS}	gN $gCOD^{-1}$	0.07****	Literature	0.07	Literature	0.07		

* Laspidou and Rittmann23.
** EPS and SMP formation kinetic parameters for autotrophic biomass are set to zero as they have been found not to affect SMP and EPS concentrations.
*** UAP and BAP are assumed to be unbiodegradable.
**** N content in EPS is assumed to be the same as in BAP.
***** Reduced from a default value of 20 to 5 in order to eliminate overshoot of substrate profile near a 10 hour mark in the batch stepping experiment (although the choice was subjective and hence the reduced value was not incorporated in the default parameter set)
Parameter fitting was performed manually (parameters adjusted by hand) during the two described calibration exercises. Some of the parameters have been calculated as a function of other parameters which had been fitted, assumed or taken from the literature.

4. Model simulation results

The biological model with its default parameters listed in Table 3 was simulated on a single completely stirred aerobic tank treatment plant configuration with an ideal separation clarifier substituting the separation membrane. The simulations were performed under steady state conditions for different dissolved oxygens (DOs), SRTs, MLSS and temperatures in order to investigate how the output SMP and EPS concentrations would differ under various operating conditions. The ranges of variability of the operational parameters were as follows: DO: 0.5-6.0 mgO_2/L, SRT: 12-250 d, MLSS: 3,000-30,000 mg/L, and temperature: 8-26 ^oC. In all simulations the non-retainable SMP fraction, f_{nr} was set to 0.5. The simulation results are shown in Fig. 4.

SMP are predicted to increase with mixed liquor volatile suspended solids (MLVSS) and decrease with SRT. The first relation is supported by the experimental results of Yigit et al. [21] who showed a linear increase in SMP vs. MLVSS. If we agree with the wide-spread and well supported hypothesis that SMP are one of the major foulants in MBR system then the second relationship is presumably correct as most of the authors claim that fouling propensity decreases with increasing SRT [26]. However, the reader needs to bear in mind that the same static SRT value can be obtained for different combinations of MLVSS and inlet COD values. Whilst MLVSS is responsible for biomass-associated SMP production and inlet organic load is responsible for utilisation-associated SMP production and these two SMP production mechanisms have different kinetics, it is possible to produce different SMP concentrations for the same values of SRT. The model predicts an increase in SMP concentration with temperature. This relationship is strong for low SRTs where SMP production is growth-related and weak for high SRTs where SMP production is biomass-related. This behaviour results from a difference in temperature dependencies of these two processes with biomass growth being more temperature sensitive than biomass decay and lysis.

The model also predicts a slight decrease in SMP concentrations at higher DO levels although this trend is very weak and increases with MLVSS setpoint. It has been reported in some literature that higher DO concentrations lead to lower elimination of SMP in MBR systems [27], but at the same time the results of other experimental studies show that mixed liquor SMP concentrations increase with DO [28]. It is generally accepted that higher DO concentrations lead to reduced amount of fouling but this can be attributed as well to better sludge filterability which depends not only on SMP but also, if not predominantly, on floc size distribution and floc geometry.

CES-ASM1 predicts that EPS concentrations will increase with MLVSS, although the content of EPS in sludge will decrease, just as observed in [21]. EPS/MLVSS ratio was also found to be in a negative proportion to SRT and temperature. For intermediate sludge ages, EPS was found to be unrelated to SRT [29], however the authors are in opinion that EPS concentrations should theoretically decrease for systems with older sludges where endogenous respiration plays a bigger role [29,30]. The relationship between EPS content and temperature is controlled by the EPS hydrolysis temperature dependency coefficient which has been initially set equal to the temperature dependency coefficient for the hydrolysis of X_S. Due to the lack of good quality literature data which could determine the exact character of the EPS vs. temperature relationship, these two coefficients have been set to an equal value of $\theta = 1.0408$. Finally, the model predicts that EPS/MLVSS ratio is independent on DO which stems from the fact that most of EPS in steady-state conditions is produced through hydrolysis, which is independent on oxygen levels.

The results indicate that DO concentration does not influence the EPS content while its effects on SMP are rather small and increase with MLVSS concentration, hence SRT. At higher SRTs it is noticeable that SMP concentration decreases with DO and this relationship is strongest for DOs between 0 and 2 mgO_2/L. SMP concentration increases with MLVSS whilst the EPS content decreases. The SMP vs. MLVSS curve is concave down which indicates that SMP content in the sludge also decreases, similarly to EPS. At higher MLVSS concentrations the bioreactor operates at lower food to mass ratio (F:M), hence growth associated production of biopolymers decreases while its uptake by biomass increases as more biomass is under starvation conditions and forced to respire on any organic substrate available. The plots could theoretically look differently if biomass associated kinetics were increased and biopolymer uptake kinetics decreased in the model. Theoretically it would then be possible to obtain curves showing increasing biopolymer contents in the biomass with increasing biomass concentrations. SMP are found to increase with temperature while EPS/MLVSS decreased. Both relationships are stronger at lower SRTs. SMP are found to decrease with SRT while EPS/MLVSS actually increase with SRT. This relationship is stronger at higher temperatures for SMP while for the EPS content the trend is not clear. It is interesting that higher SRT produced lower SMP concentrations. Such a result is due to the fact that SRT in the model was adjusted by manipulating influent COD, hence at

higher SRTs the reactor was receiving weaker sewage. If SRT was adjusted by not wasting any surplus sludge, hence increasing the sludge inventory, the results would likely have been opposite.

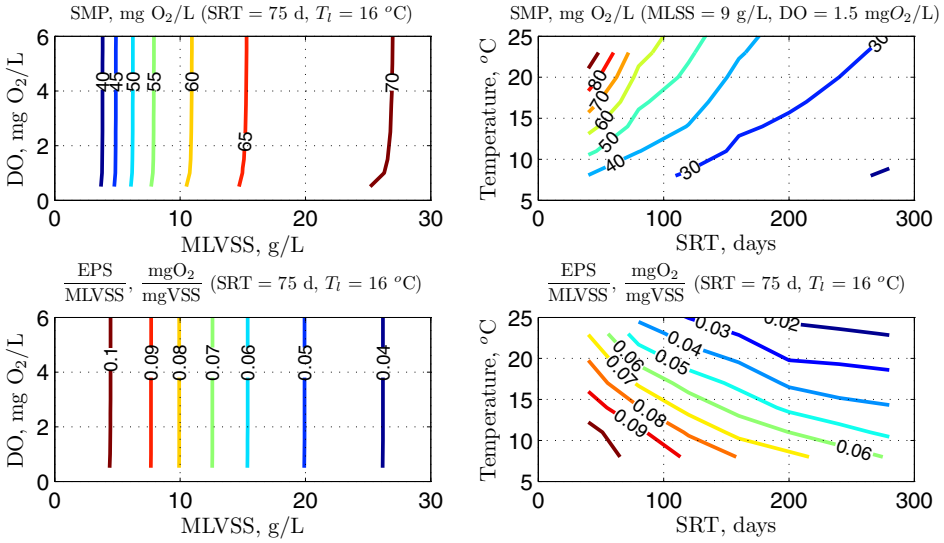


Fig. 4: CES-ASM1 predictions of SMP and EPS at different DO, MLVSS, SRT, and temperature (T_l) setpoints.

5. Conclusions

This paper presents a ASM1-based activated sludge model with SMP and EPS kinetics designed to be combined with a membrane fouling model to facilitate integrated simulation of MBRs for wastewater treatment. Contrary to some earlier developments published in literature the model is structurally correct and has been successfully calibrated on two different sets of experimental data from two very different environments. Based on the parameter values obtained from these two calibration procedures as well as the values borrowed from literature a set of default parameter values for the model was proposed and listed in Table 3. The steady-state simulation results obtained from the model using the default parameter set predicted strong positive relationship between SMP and MLVSS concentrations, and strong inverse relationship between SMP and SRT, while SMP and EPS/MLVSS were predicted to be rather insensitive to DO concentrations. EPS content in MLVSS was predicted to decrease with MLVSS, SRT and liquid temperature. Most of the above observed model behaviour is supported by experimental findings of various researchers. Although the model was not validated, it is nevertheless a good candidate for description of a bioreactor part of a MBR and it was already successfully implemented in integrated simulation study of an immersed MBR [31].

References

[1] C. S. Laspidou, B. E. Rittmann, A unified theory for extracellular polymeric substances, soluble microbial products, and active and inert biomass, Water Research 36 (2002) 2711–2720.

[2] F. Delrue, J. Choubert, A. Stricker, M. Sperandino, M. Miletton-Peuchot, Y. Racault, Modelling a full scale membrane bioreactor using Activated Sludge Model No.1: challenges and solutions, Water Science and Technology 62 (2010) 2205–2217.

[3] Z. Wang, Z. Wu, S. Tang, Extracellular polymeric substances (EPS) properties and their effects on membrane fouling in a submerged membrane bioreactor, Water Research 43 (2009) 2504–2512.

[4] J. Wu, C. He, Y. Zhang, Modelling of membrane fouling in a submerged membrane bioreactor by considering the role of solid, colloidal and soluble components, Journal of Membrane Science 397-398 (2012) 102–111.

[5] S. G. Lu, T. Imai, M. Ukita, M. Sekine, T. Higuchi, M. Fukagawa, A model for membrane bioreactor process based on the concept of formation and degradation of soluble microbial products, Water Research 35 (2001) 2038–2048.

[6] K. P. Oliveira-Esquerre, H. Narita, N. Yamato, N. Funamizu, Y. Watanabe, Incorporation of the concept of microbial product formation into ASM3 and the modelling of a membrane bioreactor for wastewater treatment, Brazilian Journal of Chemical Engineering 23 (2006) 461–471.
[7] Y. T. Ahn, Y. K. Choi, H. S. Jeong, S. R. Chae, H. S. Shin, Modeling of extracellular polymeric substances and soluble microbial products production in a submerged membrane bioreactor at various SRTs., Water Science and Technology 53 (2006) 209–216.
[8] B.-J. Ni, B. E. Rittmann, F. Fang, J. Xu, Long-term formation of microbial products in a sequencing batch reactor, Water Research 44 (2010) 3787–3796.
[9] T. Jiang, S. Myngheer, D. J. D. Pauw, H. Spanjers, I. Nopens, M. D. Kennedy, G. Amy, P. A. Vanrolleghem, Modelling the production and degradation of soluble microbial products (SMP) in membrane bioreactors (MBR), Water Research 42 (2008) 4955–4964.
[10] T. Janus, Modelling and Simulation of Membrane Bioreactors for Wastewater Treatment, Ph.D. thesis, De Montfort University, School of Engineering, Media and Sustainable Development, Leicester, UK, 2013.
[11] T. Janus, B. Ulanicki, Modelling SMP and EPS formation and degradation kinetics with an extended ASM3 model, Desalination 261 (2010) 117–125.
[12] J. B. Copp, The COST simulation benchmark - description and simulator manual., Luxembourg: Office for Official Publicatios of the European Communities, 2002. ISBN: 92-894-1658-0.
[13] T. Maere, B. Verrecht, S. Moerenhout, S. Judd, I. Nopens, BSM-MBR: A benchmark simulation model to compare control and operational strategies for membrane bioreactors, Water Research 45 (2011) 2181–2190.
[14] M. Henze, C. Grady, W. Gujer, G. Marais, T. Matsuo, Activated Sludge Model No. 1, Technical Report No. 1, IAWQ Scientific and Technical Report, London, 1987.
[15] S. F. Aquino, D. C. Stuckey, Integrated model of the production of soluble microbial products (SMP) and extracellular polymeric substances (EPS) in anaerobic chemostats during transient conditions, Biochemical Engineering Journal 38 (2008) 138–146.
[16] A. Menniti, E. Morgenroth, Mechanisms of SMP production in membrane bioreactors: Choosing an appropriate mathematical model structure, Water Research 44 (2010) 5240–5251.
[17] R. Leudeking, E. Piret, A kinetic study of lactic acid fermentation., Journal of Biochemical and Microbiological Technology and Engineering 1 (1959) 393–412.
[18] J. W. Cho, K. H. Ahn, Y. Seo, Y. Lee, Modification of ASM No.1 for a submerged membrane bioreactor system: Including the effects of soluble microbial products (SMP) on membrane fouling, Water Science and Technology 47 (2001) 177–181.
[19] M. Henze, W. Gujer, T. Mino, M. van Loosdrecht, Activated sludge models ASM1, ASM2, ASM2d and ASM3, IWA Publishing, 2000.
[20] K. M. Hsieh, G. A. Murgel, L. W. Lion, M. L. Shuler, Interactions of microbial biofilms with toxic trace metals: 2. prediction and verification of an integrated computer model of lead (II) distribution in the presence of microbial activity., Biotechnology & Bioengineering 44 (1994) 232–239.
[21] N. Yigit, I. Harman, G. Civelekoglu, H. Koseoglu, N. Cicek, M. Kitis, Membrane fouling in a pilot-scale submerged membrane bioreactor operated under various conditions, Desalination 231 (2008) 124–132. Selected Papers Presented at the 4th International IWA Conference on Membranes for Water and Wastewater Treatment, 15-17 May 2007, Harrogate, UK. Guest Edited by Simon Judd.
[22] K. M. Hsieh, G. A. Murgel, L. W. Lion, M. L. Shulera, Interactions of microbial biofilms with toxic trace metals: 1. observation and modeling of cell growth, attachment, and production of extracellular polymer., Biotechnology & Bioengineering 44 (1994) 219–231.
[23] C. S. Laspidou, B. E. Rittmann, Non-steady state modeling of extracellular polymeric substances, soluble microbial products, and active and inert biomass, Water Research 36 (2002) 1983–1992.
[24] S. Aquino, D. Stuckey, Production of soluble microbial products (SMP) in anaerobic chemostats under nutrient deficiency, Journal of Environmental Engineering 129 (2003) 1007–1014.
[25] D. Noguera, N. Araki, B. Rittmann, Soluble microbial products (SMP) in anaerobic chemostats., Biotechnology & Bioengineering 44 (1994) 1040–7.
[26] A. Drews, M. Vocks, U. Bracklow, V. Iversen, M. Kraume, Does fouling in MBRs depend on SMP?, Desalination 231 (2008) 141–149. Selected Papers Presented at the 4th International IWA Conference on Membranes for Water and Wastewater Treatment, 15-17 May 2007, Harrogate, UK. Guest Edited by Simon Judd; and Papers Presented at the International Workshop on Membranes and Solid-Liquid Separation Processes, 11 July 2007, INSA, Toulouse, France. Guest edited by Saravanamuthu Vigneswaran and Jaya Kandasamy.
[27] A. Drews, J. Mante, V. Iversen, M. Vocks, B. Lesjean, M. Kraume, Impact of ambient conditions on SMP elimination and rejection in MBRs, Water Research 41 (2007) 3850–3858.
[28] L. Holakoo, G. Nakhla, A. S. Bassi, E. K. Yanful, Long term performance of MBR for biological nitrogen removal from synthetic municipal wastewater, Chemosphere 66 (2007) 849–857.
[29] B. Q. Liao, D. G. Allen, I. G. Droppo, G. G. Leppard, S. N. Liss, Surface properties of sludge and their role in bioflocculation and settleability, Water Research 35 (2001) 339–350.
[30] V. Gulas, M. Bond, L. Benefield, Use of extracellular polymers for thickening and dewatering activated sludge., Journal of Water Pollution Control Federation 51 (1979) 798–807.
[31] T. Janus, Integrated mathematical model of a {MBR} reactor including biopolymer kinetics and membrane fouling, Procedia Engineering 70 (2014) 882 – 891. 12th International Conference on Computing and Control for the Water Industry, {CCWI2013}.