1 MATERIALS AND METHODS

1.1 Simulation of continuous model in a continuous PAnMBR

The resulting kinetic expressions were used in the development of a continuous PAnMBR model. As previously demonstrated, the concentration of the bioavailable sCOD in medium strength domestic wastewater is insufficient for the system to achieve total nitrogen and total phosphorous discharge limits (Hülsen et al., 2015). To achieve full removal, additional sCOD is required.

The simulation was therefore carried out to highlight this additional requirement, while at the same time, establishing system's response to considerable and minimal perturbations in the influent characteristics. Dynamic influent data were obtained from Gernaey, et al., 2014, and adapted to the typical concentrations of primary influent reported by Hülsen et al., 2014. Based on the average influent characteristics and an HRT of 24 h, volumetric loading rate (VLR) of and a solid retention time (SRT) of 4 d, a reactor volume of 21 m^3 was imposed.

Comment [TH1]: Id use mg and m3 but you might as well leave it as it looks like you used your units for modelling

The simulation and subsequent data processing were performed using a commercial software package (MATLAB R2015a, The MathWorks Inc., Natick, MA). As the system of equations is stiff, the resolution of the ordinary differential equations was carried out using ODE15s. The model was simulated for 460 days with 50 day periods of low ( ), medium ( ) and high ( ) sCOD concentrations. Other soluble organics ( ) were fixed with only acetate ( ) modified. The general design equations for both solid (X) and soluble (S) species (i) are as follows, with the explanation of variable names available in Table 1.

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Table 1: Explanation of variables and values used in continuous PAnMBR simulation

Variable	Value	Unit
V (reactor volume)		
(concentration of soluble species)	Dynamic influent data	*
(concentration of particulate species)	Dynamic influent data	
(feed flow rate)		
(concentration of soluble	Dynamic influent	*

species in feed)	data	
(concentration of particulate species in feed)	Dynamic influent data	
(liquid flow rate out)		
(solid flow rate out)		
(rate of reaction of species)	N/A	*
*		

The different periods were simulated as listed in Table 2;

Table 2: sCOD concentrations over different periods for the continuous PAnMBR simulation

Condition	Value	Time (d)
Low sCOD		[150;200), [250;300), [350;450), [500;600)
Medium sCOD		[200;250), [450;500)
High sCOD		[300;350)

Comment [TH3]: Id use mg and m3 but you might as well leave it as it looks like you used your units for modelling

Comment [TH4]: How much is low, medium and high, give numbers

The results from the simulation were balanced over COD, N, P and C, and have been included in the supplementary material. The influent data and effluent results are displayed as 24 hour moving averages with 95% confidence intervals.

Gernaey, K. V., Flores-Alsina, X., Rosen, C., Benedetti, L., Jeppsson, U., 2011. Dynamic influent pollutant disturbance scenario generation using a phenomenological modelling approach. Environ. Model. Softw. 26, 1255–1267. doi:10.1016/j.envsoft.2011.06.001

Hülsen, T., Batstone, D.J., Keller, J., 2014. Phototrophic bacteria for nutrient recovery from domestic wastewater. Water Res. 50, 18–26. doi:10.1016/j.watres.2013.10.051

Hülsen, T., Barry, E.M., Lu, Y., Puyol, D., Batstone, D.J., 2015. Low temperature treatment of domestic wastewater by purple phototrophic bacteria: performance, activity, and community. Water Res. (in submission).

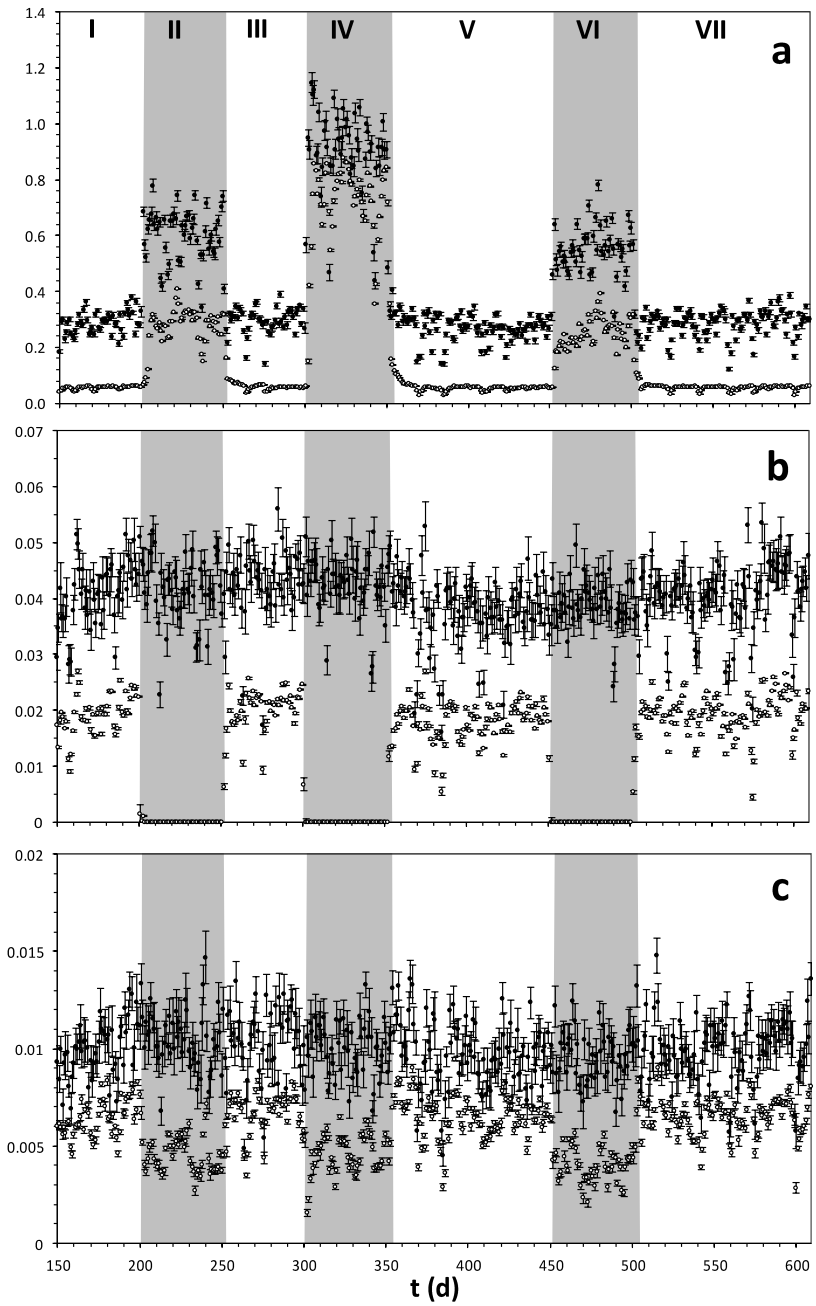
MATLAB Release 2015a, The MathWorks, Inc., Natick, Massachusetts, United States.

2 DISCUSSION

2.1 Dependence of system on influent characteristics

2.1.1 Addition of acetate as sCOD

The model indicates different sCOD removal efficiencies for the particular periods of operation. For periods (I), (III), (V), and (VII), which correspond to no additional acetate in the system, the mean removal efficiency is . The remaining sCOD in the system can be almost entirely attributed to the presence of non-biodegradable sCOD, accounting for 97% of the effluent sCOD. During periods (II) and (VI), the removal efficiency is reduced as acetate is added slightly in excess in order to satisfy requirements for nitrogen and phosphorus removal. The mean sCOD removal efficiency during these periods is 45.0% ± 0.6%. In this case, the fraction of non-biodegradable sCOD in the effluent is 48.0% ± 0.4%. Period (IV) relates to the case where excessive additional acetate is added. This component of the simulation aims to show the reaction of the system to a higher load of sCOD entering a wastewater treatment plant. The removal efficiency is 1.0%. This can be explained by the fact that the scaling factor to increase the influent acetate concentration was also applied to the composite particulates concentration being fed to the PAnMBR. The composite biomass accumulates within the reactor, but is also hydrolysed, leading to an increase in sCOD concentration within the reactor. The composite particulate concentration was increased in order to approximate industries with high particulate concentrations or periods after heavy rainfall.


I
II
III
IV
V
VI
VII
a
b
c
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.07
0.06
0.05
0.04
0.03
0.02
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150
200
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t (d)

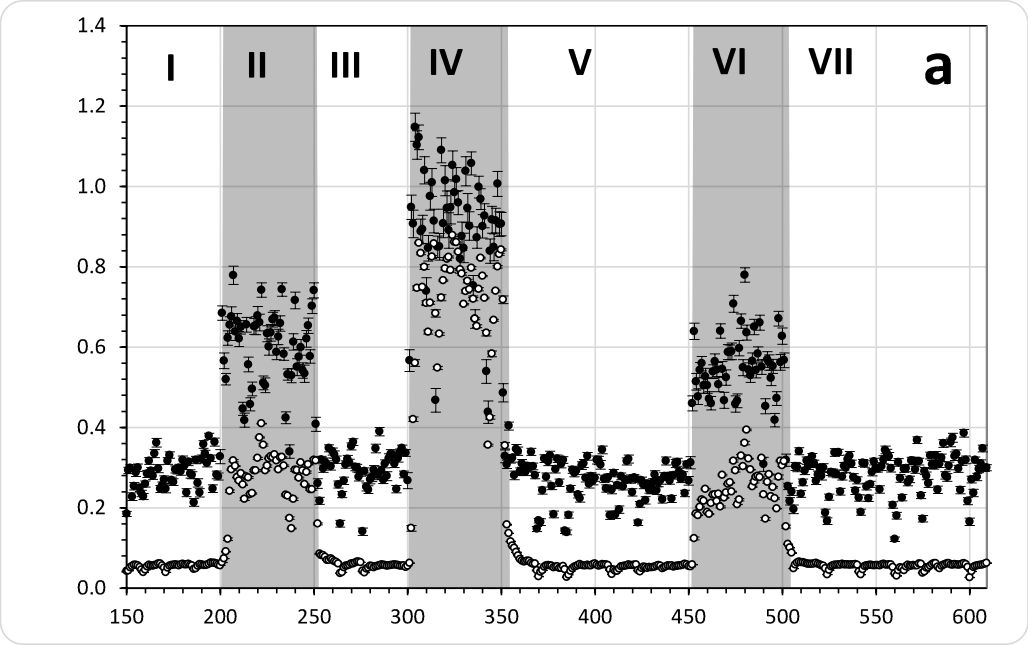

Figure 1: sCOD influent (●) and effluent concentrations (○) over time for PAnMBR simulation. All points represent a one day moving average and include 95% confidence intervals for the 24 hour time period. Period (I) shows sCOD removal with no acetate addition for a 50 day period. Similarly, periods (III), (V) and (VII) operate at the same conditions for 50, 100 and 100 days respectively. Periods (II) and (VI) represent operation with added. A higher concentration of sCOD (acetate added) is shown in Period (IV).

2.1.2 Uptake of nitrogen and phosphorus

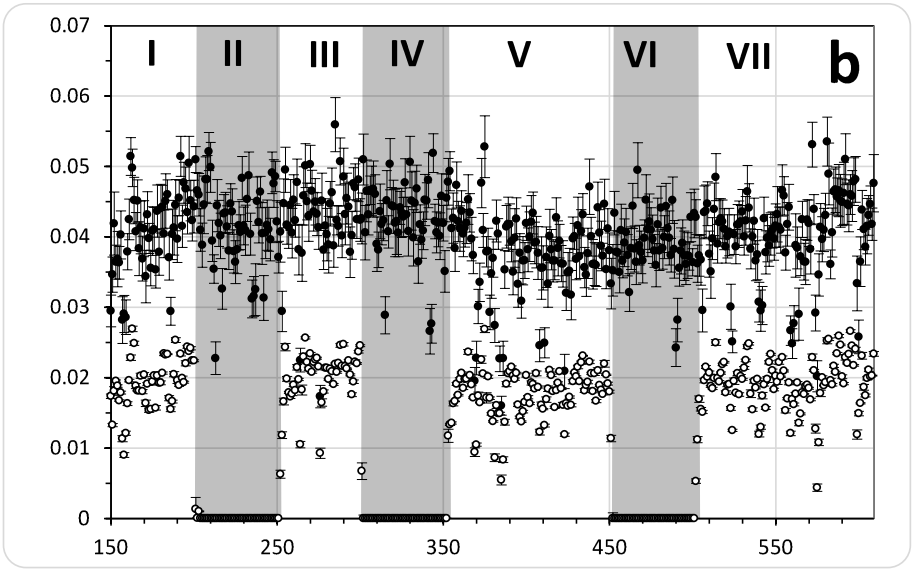

Figure 2: NH_4-N influent (●) and effluent concentrations (○) over time for the PAnMBR continuous simulation. A 24 hour moving average and 95% confidence interval are displayed for each data point. Periods (I), (III), (V), and (VII) represent the cases where there was no additional acetate added. Periods (II) and (VI) represent operation with added. A higher concentration of sCOD (acetate added) is added in Period (IV).

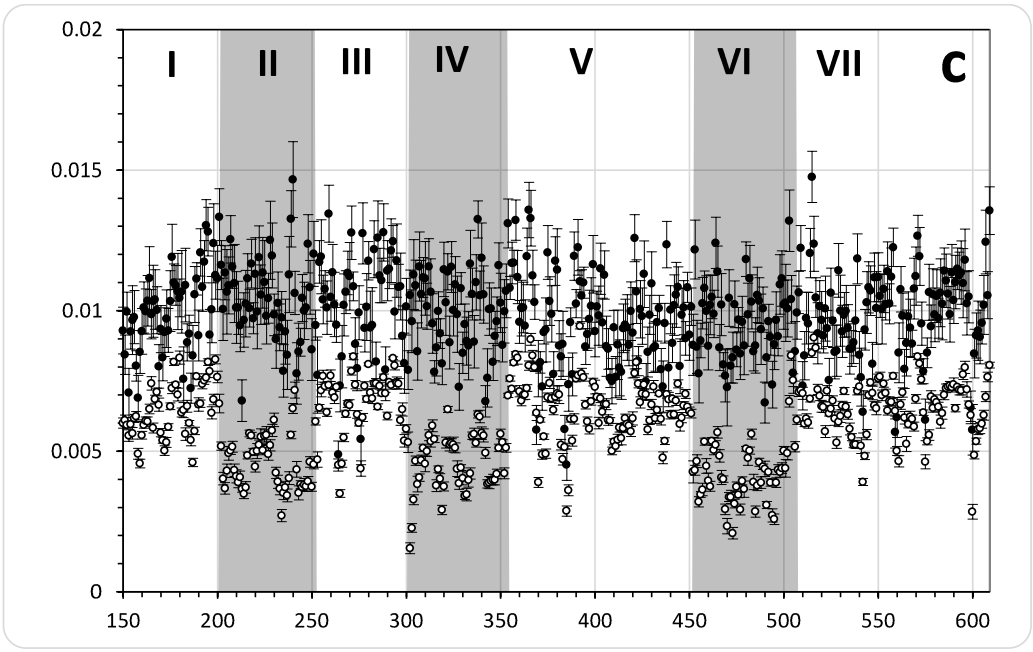

Figure 3: PO_4-P influent (●) and effluent concentrations (○) over time for the PAnMBR continuous simulation. A 24 hour moving average and 95% confidence interval are displayed for each data point. Periods (I), (III), (V), and (VII) represent the cases where there was no additional acetate added. Periods (II) and (VI) represent operation with added. A higher concentration of sCOD (acetate added) is added in Period (IV).

2.1.3 Biomass Production

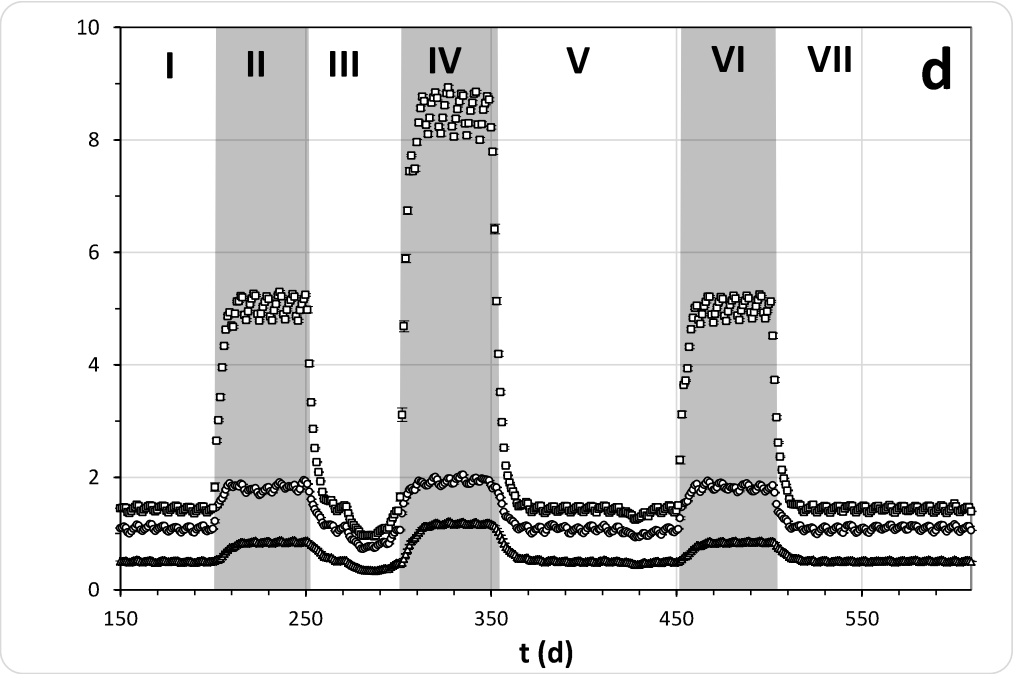

Figure 4: Particulate COD effluent including PPB (○), composite biomass (□) and inert particulates (Δ) over time for the PAnMBR continuous simulation. Each data point represents a 24 hour moving average and includes 95% confidence intervals. Periods (I), (III), (V), and (VII) represent the cases where there was no additional acetate added. Periods (II) and (VI) represent operation with added. A higher concentration of sCOD (acetate added) is shown in Period (IV).

Production of X by the increase/decrease of sCOD addition, include mass balances

X =biomass production??

For the certain periods

X production is for no addition of organics, the mass balance would be interesting. How much influent COD goes to X and how much leaves the reactor. Does this depend on CID addition?? by itself does not say anything, need to ralte to COD influent load, same below. A fraction of CODin converted to X would say something, so maybe ,mass balance: how much of CODin goes to X, effluent and what cannot be accounted for –loss.

X production is for medium addition of organics

X production is for high addition of organics

The addition of acetate COD is as follows;

for medium addition

for high addition

Period	Xppb	Xc	Xi	X_T	%PPB	%Xc	%Xi
I	1.09	1.44	0.51	3.03	35.85	47.44	16.71
CI95%	0.011555465	0.011423905	0.003119644	0.009552776			
II	1.76	4.73	0.79	7.28	24.21	64.88	10.91
CI95%	0.043683983	0.230209484	0.028953778	0.136312164			
III	1.05	1.60	0.50	3.16	33.22	50.79	15.99
CI95%	0.082685335	0.263777677	0.043272953	0.161542643			
IV	1.86	7.88	1.07	10.80	17.19	72.94	9.87
CI95%	0.056810602	0.465604335	0.058910736	0.272937915			
V	1.12	1.74	0.56	3.43	32.74	50.91	16.35
CI95%	0.052725272	0.320889538	0.042553856	0.18935054			
VI	1.75	4.68	0.79	7.23	24.27	64.79	10.94
CI95%	0.051428617	0.24108808	0.029545248	0.143342581			
VII	1.13	1.61	0.54	3.29	34.48	49.08	16.44
CI95%	0.041899467	0.176930418	0.021774532	0.105726169			

2.1.4 Limitations of the Model

No gas phase reactions

No irradiance

No inclusion of phosphates

In reality, losses occur, but this model includes no empirical loss terms

Comment [TH5]: I would mark the different periods to facilitate interpretation of this fig without scrolling back to table 2 e.g. like ...

Period	Cef(%)	N ef(%)	P ef(%)
I	80.56	52.17	34.61
CI95%	0.73476899	1.68673989	2.43072975

II	55.39	98.42	55.59
CI95%	3.32987855	2.13528746	2.32123061
III	77.35	55.02	34.50
CI95%	3.10136	3.82669641	3.24062304
IV	22.05	97.92	53.40
CI95%	6.18134717	2.76566229	3.00123301
V	75.74	54.16	32.52
CI95%	4.85318236	3.24218464	2.87686257
VI	55.93	97.61	56.91
CI95%	3.14255766	2.8427909	2.46643076
VII	78.97	53.53	33.56
CI95%	1.90694422	2.87046405	2.97305593

SUPPLEMENTARY MATERIAL

The model was developed according to a mass balance over a continuously stirred tank reactor, with a membrane completely separating the solids from the fluid stream. Influent data were generated from the ASM dynamic influent generator (Gernaey, et al., 2014). The generic design equations for both soluble (S) and particulate (X) concentrations of species *j* are as follows;

The explanation of each variable is presented in Materials and Methods. The rate equations are those given in Table XXX. The stoichiometric coefficients and parameters used in the simulation were quantified in Table XXXX.

The simulation was carried out using Matlab Release 2015a (The Mathworks, Natick, MA). The ODE integrator used throughout the simulations was the standard ODE15s in Matlab. This was chosen as this is a stiff system, and numerical diffusion would have occurred if any other standard integrator was used.

The simulation was run for a 460 day period. A reactor volume of 21 000 L was chosen such that the average hydraulic retention time (HRT) was 24 hours. The solids retention time (SRT) as imposed at 4 days. The HRT and SRT were chosen because these were conditions at which the lab scale PAnMBR was operated (Cite Tim Cold Paper).

Data were analysed using Matlab Release 2015a. For each input and state variable, a t-distribution 95% confidence interval was carried out (n = 39754). Each variable stated in this paper has undergone the same statistical analysis on the same number of datapoints. A script was written in Matlab in order to batch process these results.

The data were presented as 24 hour moving averages, with seven distinct periods of varying added acetate concentrations. These have been described in detail in Table 2. The dynamic mass balances over TCOD, C, N and P gave the following results.

Table 3: Dynamic mass balances over C, N, P and TCOD

Substrate	**Average relative error**
C	0
N	0.01
P	0.08
TCOD	0

2.1.5 References: Supplementary Information

Gernaey, K. V., Flores-Alsina, X., Rosen, C., Benedetti, L., Jeppsson, U., 2011. Dynamic influent pollutant disturbance scenario generation using a phenomenological modelling approach. Environ. Model. Softw. 26, 1255–1267. doi:10.1016/j.envsoft.2011.06.001