

Colloids, flocculation and carbon capture – a comprehensive plant-wide model

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ABSTRACT

The implementation of carbon capture technologies such as high-rate activated sludge (HRAS) systems are gaining interests in water resource and recovery facilities (WRRFs) to minimize carbon oxidation and maximize organic carbon recovery and methane potential through biosorption of biodegradable organics into the biomass. Existing activated sludge models were developed to describe chemical oxygen demand (COD) removal in activated sludge systems operating at long solids retention times (SRT) (i.e. 3 days or longer) and fail to simulate the biological reactions at low SRT systems. A new model is developed to describe colloidal material removal and extracellular polymeric substance (EPS) generation, flocculation, and intracellular storage with the objective of extending the range of whole plant models to very short SRT systems. In this study, the model is tested against A-stage (adsorption) pilot reactor performance data and proved to match the COD and colloids removal at low SRT. The model was also tested on longer SRT systems where effluents do not contain much residual colloids, and digestion where colloids from decay processes are present.

Key words | biosorption, contact stabilization, organic substrate, oxidation, process modelling

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LIST OF ACRONYMS

AAA alternating activated adsorption process

AB adsorption bio-oxidation

CS contact-stabilization

EPS extracellular polymeric substances

HRAS high-rate activated sludge

WRRF water resource and recovery facilities

AHO carbon adsorption heterotrophic organisms
[g COD/m³]

OHO ordinary heterotrophic organisms [g COD/m³]
S_{B,mono} readily biodegradable substrate as monomers
[g COD/m³]

S_{B,poly} readily biodegradable substrate as polymers
[g COD/m³]

VFA volatile fatty acids [g COD/m³]

f_{EPS,VSS} EPS content of the sludge [g COD/gVSS]

X_{BIO} sum of all active biomasses [g COD/m³]

$\eta_{\text{FLOC,Process}}$ flocculation reduction factor due to process
specifics [- in the range 0–1]

INTRODUCTION

The implementation of carbon capture technologies such as the A-stage of the adsorption bio-oxidation (AB) process and contact-stabilization (CS) as a form of high-rate activated sludge (HRAS) systems are gaining interests in water resource and recovery facilities (WRRFs). The intent of these systems is to minimize carbon oxidation and maximize organic carbon recovery and biogas potential (28% to 42% (Rahman *et al.* 2019)) through biosorption of degradable organics into the biomass at very low solids retention time (SRT of 0.1–1.0 d) and hydraulic retention time (HRT of 0.5–1.0 h).

The removal of organics (measured as COD) in the A-stage can be attributed to intracellular storage and oxidation by heterotrophic bacteria together with the bioflocculation of suspended solids and colloids. The stored, flocculated and adsorbed organic material in the sludge can be removed in the settler without having been metabolized by bacteria (Smitshuijzen *et al.* 2016). These processes are taking place in a short period of time and their efficiency is linked to SRT, extracellular polymeric substances (EPS) and dissolved oxygen (DO) levels in the reactor (Jimenez *et al.* 2015; Rahman *et al.* 2016; Rahman *et al.* 2017).

The modelling of activated sludge processes, particularly the chemical oxygen demand (COD) transformation, has significantly evolved towards fundamental principles in the past decades from simple single-substrate models to more complex multiple-substrate models involving the description of oxidation, hydrolysis and storage phenomenon (Dold *et al.* 1980; Sin *et al.* 2005). However, these models were developed to describe COD removal in systems operating at long solids retention times (SRT) (i.e. 3 days or longer) where the readily biodegradable organic substrate (S_B) can be modelled as single substrate by a single removal kinetics, and the capture of slowly biodegradable substrate (particulate, X_B ; and colloidal, C_B) by flocculation is not the rate limiting process, hence, it can be ignored in the models (Haider *et al.* 2003; La Motta *et al.* 2003). However, in high-rate systems (HRAS) as those employed in the AB process where the SRT may be well below one day, these assumptions with respect to organic substrate transformations are no longer applicable. In addition, for systems that include longer SRT processes, such as membrane bioreactors, biofilm-based systems (i.e. MBBRs, trickling filters) and digesters, flocculation of colloidal particles must be described by the same model to accurately describe the fate of organics throughout the whole plant.

By critically evaluating previous models and a wide range of experimental data from several carbon capture technologies, a new plant-wide mechanistic model was developed to describe colloidal material and EPS generation, flocculation, and intracellular storage in all typical units of a WRRF.

MODEL DEVELOPMENT

Existing high-rate activated sludge systems models

Based on a literature review, few models have been developed for HRAS processes, all extending the ASM1 model.

Haider *et al.* (2003) introduced two readily biodegradable substrates, one being consumed with a higher growth rate in A-stage. However, despite the experimental results of this study showing that HRAS processes select fast growing biomass, a single heterotrophic biomass was considered. Moreover, no colloidal material capture was considered in this model.

Smitshuijzen *et al.* (2016) proposed a model based on ASM1 without adding any new state variables for COD components. A fixed fraction of particulate substrate was considered absorbed in A-stage to count for colloidal removal. Kinetics were adapted for A-stage modelling but were not valid for a whole plant model.

Nogaj *et al.* (2015) model included EPS as a state variable, two readily biodegradable substrates for a single biomass, the production of storage products and the adsorption of colloidal material. This model required assumptions on EPS production yield, kinetics of production and degradation which affect the concentration of active biomass. In addition, the variability in EPS measurements associated with the type of methods used would be an issue for model calibration.

Model description

A plant-wide model (Sumo2) by Dynamita (Dynamita 2016) considering typical biological and physico-chemical reactions of activated sludge and anaerobic digestion was used as the 'base model'. This base model was modified to include the required components and processes in accordance with the critical review of existing models and experimental data, as summarized in Figure 1. The following is a list of model modifications with a brief description:

- Readily biodegradable substrate (S_B) is split into monomers and polymers ($S_{B,mono}$ and $S_{B,poly}$) as reported in Haider *et al.* (2003) and in Nogaj *et al.* (2015). $S_{B,mono}$ and $S_{B,poly}$ fractions depend on the wastewater characteristics and has been used here as calibration parameters based on A-stage residual rbCOD.
- A new fast growing biomass, carbon adsorption heterotrophic organisms (AHO) is added to help describe processes specific to HRAS. To reproduce the lower mineralization or loss of COD content observed in A-stage processes (Jimenez *et al.* 2015), this biomass stores $S_{B,mono}$ and volatile fatty acids (S_{VFA}) in storage product (X_{STO}), while the Ordinary Heterotrophic Organisms (OHO) consume only $S_{B,poly}$ and have a lower growth rate. The storage process is sensitive to DO conditions, consequently a reduction factor for the kinetic rate is

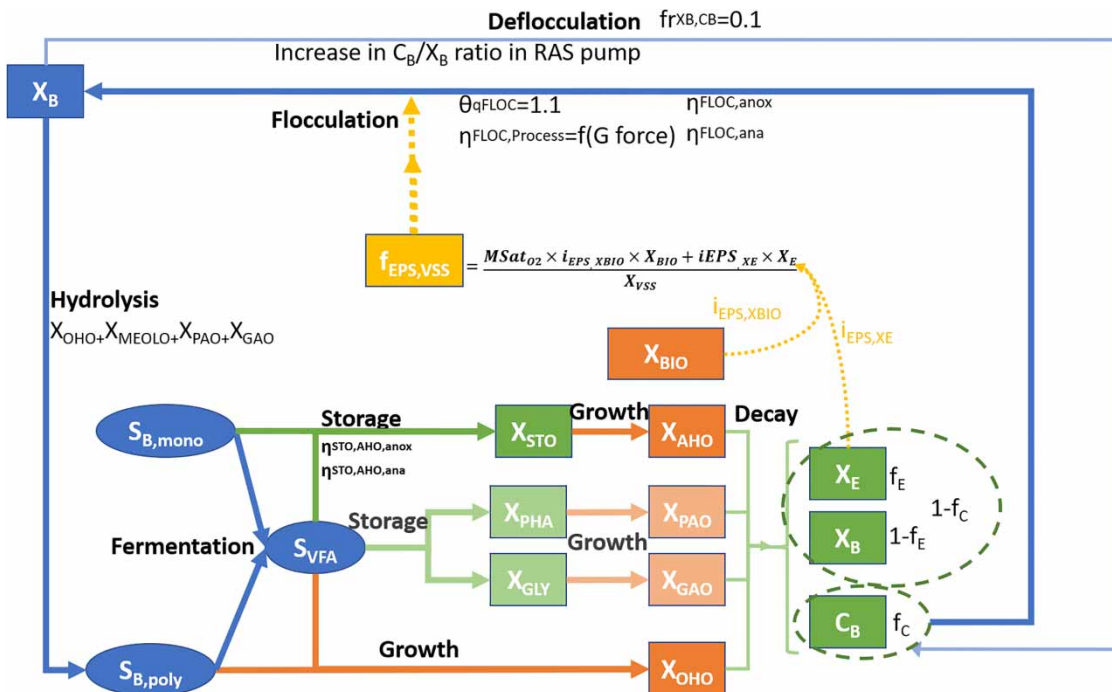


Figure 1 | Biological processes added and modified for the removal and capture of organics in the modified model.

used under anoxic and anaerobic conditions ($\eta_{\text{STO,AHO,anoX}}$ and $\eta_{\text{STO,AHO,ana}}$, respectively).

- Hydrolysis is mediated only by heterotrophic organisms (OHO, MEOLO (Methylotrophs), phosphorus accumulating organisms (PAO) and glycogen accumulating organisms (GAO)) with lower growth rates to simulate the low hydrolysis observed in A-stage processes.
- Decay processes produce a fraction (f_c) of colloidal biodegradable substrate (C_B) to model the high colloidal material content observed in digesters.
- The modified model incorporates calculation of EPS content of the sludge ($f_{\text{EPS,VSS}}$) as a flocculation agent

is reduced (Nogaj et al. 2015). Therefore, Monod saturation functions and reduction factors for anoxic and anaerobic conditions are used in the calculation ($\eta_{\text{FLOC,anoX}}$ and $\eta_{\text{FLOC,ana}}$ respectively) (Equation (1)). For lack of information and to keep the model simple as well as limiting the numbers of new parameters, it has been decided at this stage not to distinguish the impact of different biomasses in the EPS production. The role of endogenous decay products in the EPS calculation is considered in anticipation of the use of this plant-wide model in predicting granule formation, as an indicator of floc densification.

$$f_{\text{EPS,VSS}} = \left(\frac{MSat_{\text{O}_2,\text{KO}_2,\text{EPS}} + \eta_{\text{EPS,anoX}} \times MSat_{\text{NO}_2,\text{KNO}_2,\text{EPS}} \times \text{Minh}_{\text{SO}_2,\text{KO}_2,\text{EPS}} + \eta_{\text{EPS,anoX}} \times MSat_{\text{NO}_3,\text{KNO}_3,\text{EPS}} \times \text{Minh}_{\text{NO}_2,\text{KNO}_2,\text{EPS}} \times \text{Minh}_{\text{SO}_2,\text{KO}_2,\text{EPS}} + \eta_{\text{EPS,ana}} \times \text{Minh}_{\text{NO}_3,\text{KNO}_3,\text{EPS}} \times \text{Minh}_{\text{NO}_2,\text{KNO}_2,\text{EPS}} \times \text{Minh}_{\text{SO}_2,\text{KIO}_2,\text{EPS}}}{X_{\text{VSS}}} \right) \times i_{\text{EPS,XBIO}} \times X_{\text{BIO}} + i_{\text{EPS,XE}} \times X_{\text{E}} \quad (1)$$

that directly affect the flocculation kinetic rate. This calculated variable is based on the sum of calculated EPS content of biomasses ($i_{\text{EPS,XBIO}} \times X_{\text{BIO}}$) and of particulate endogenous decay products ($i_{\text{EPS,XE}} \times X_{\text{E}}$) related to the particulate VSS (X_{VSS}). The EPS content of biomasses (X_{BIO}) depends on electron acceptor conditions, meaning that under low DO, EPS production

where $MSat_{\text{O}_2,\text{KO}_2,\text{EPS}}$ and $\text{Minh}_{\text{SO}_2,\text{KO}_2,\text{EPS}}$ are respectively the Monod saturation and inhibition terms for O_2 ; $MSat_{\text{NO}_2,\text{KNO}_2,\text{EPS}}$ and $\text{Minh}_{\text{NO}_2,\text{KNO}_2,\text{EPS}}$ are respectively the Monod saturation and inhibition terms for NO_2 ; $MSat_{\text{NO}_3,\text{KNO}_3,\text{EPS}}$ and $\text{Minh}_{\text{NO}_3,\text{KNO}_3,\text{EPS}}$ are respectively the Monod saturation and inhibition terms for NO_3 ; $i_{\text{EPS,XBIO}}$ and $i_{\text{EPS,XE}}$ are respectively the EPS

content of the biomass and the endogenous decay products and X_{VSS} is the particulate volatile suspended solids. The calculated extracellular polymeric substance content of the sludge ($f_{EPS,VSS}$) is an indicator of EPS production. However, the calculated values should not be compared directly to EPS measurements as results available in the literature depend on the analysis method used by different authors. In this study, the calibration has been done based on EPS measurement data obtained with cation exchange resin (CER) extraction method developed by Frølund *et al.* (1996); Jimenez *et al.* (2015).

- The kinetic rates of flocculation processes are first order reactions that are found to be well correlated with the total biomass concentration (X_{BIO}) as described by Jimenez *et al.* (2005), using a fraction: the calculated EPS content of the sludge ($f_{EPS,VSS}$). As flocculation is a surface reaction on flocs, the kinetic rates are considered to saturate as the amount of colloidal material becomes large in proportion to the biomass, therefore the kinetic rates include a Monod ratio saturation term for colloidal biodegradable substrate to biomasses ($MR_{sat_{CB,XBIO,KFLOC}}$).

Furthermore, the flocculation rate is sensitive to temperature and to mixing intensity (G). Due to lack of measured data on the impact of aeration and mixing energy and equipment on deflocculation, a flocculation reduction factor ($\eta_{FLOC,Process}$ in the range 0–1) is introduced into the kinetic rate expression to account for deflocculation processes. The flocculation reduction factor varies in each reactor depending on the aeration and mixing technology. Initial values for this parameter are proposed by the authors, and can be adjusted to the case-study: $\eta_{FLOC,Process} = 0.1$ for fine bubbles, 0.25 for coarse bubble, 0.5 for anoxic mixed processes, 0.75 for anaerobic processes, 0.9 for an upflow sludge blanket and 1 for a flocculation tank. Equation (2) represents the flocculation rate calculation considered in the model.

$$r_{FLOC} = q_{FLOC,T} \times X_{BIO} \times f_{EPS,VSS} \times \eta_{FLOC,Process} \times MR_{sat_{CB,XBIO,KFLOC}} \quad (2)$$

- An empirical pump process unit is implemented to simulate the deflocculation processes occurring in pumps. The factor for the increase in C_B/X_B and C_U/X_U ratio ($fr_{CB_{XB}}$ and $fr_{CU_{XU}}$, respectively) can be adjusted depending on the pump technology.

The main parameters introduced in this new model are presented in Table 1 with their default values

determined by the calibration study presented hereafter. The full Gujer matrix of the model is available as supplementary material (<http://www.dynamita.com/public/models/Sumo2C.xlsm>).

RESULTS AND DISCUSSION

The model was first calibrated to a HRAS (A-stage) pilot-scale reactor treating municipal raw wastewater operated at Laboratory of University of New Orleans (UNO) and the reactor was operated at an SRT and HRT range of 0.3–2 d and 0.5–1.1 hours, respectively (Jimenez *et al.* 2015). Later, the calibrated model was validated on Blue Plains Carbon management pilot reactor treating chemically enhanced primary treatment effluent (CEPT) and operated at an SRT range of 0.3–1.4 d (Rahman *et al.* 2016). Subsequently, the model was applied in different full-scale plant configurations such as Rochester (MN) Wastewater Treatment Plant (WWTP) A-stage and alternating activated adsorption process (AAA) Rotenburg WWTP A-stage to verify the performance of the model.

Model calibration: UNO A-stage pilot case study

The detailed description of the University of New Orleans (UNO) A-stage pilot can be found in Jimenez *et al.* (2015, 2005) and the configuration is presented in Figure 2. The results used for this calibration exercise were taken from Jimenez *et al.* (2015), in which effect the of SRT and DO on the system was investigated separately.

SRT effect

The SRT in the pilot plant was varied between 0.3 days and 2 days by continuously wasting settled mixed liquor from the return activated sludge (RAS) line. The SRT calculation neglects the biomass in the sedimentation tank. The main calibration was performed on this set of data. The EPS content of X_{BIO} and X_E ($i_{EPS,XBIO}$ and $i_{EPS,XE}$, respectively) were calibrated to fit the EPS curve as a function of SRT (Figure 3(a)); parameters for AHO and OHO growth were calibrated to fit observed soluble COD removal (Figure 3(b)) and flocculation parameters were calibrated to fit observed colloidal removal (Figure 3(c)). The parameters used in the model are listed in Table 1. All parameters have been calibrated on this data set. The model was found to be very sensitive to influent

Table 1 | Main parameters for OHO and AHO growth, EPS calculation and flocculation

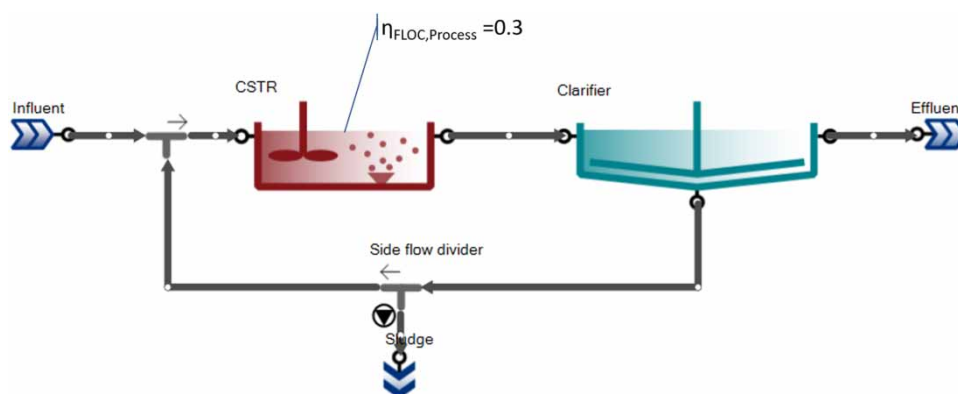
Parameter	Sumo2	Sumo2C	
	OHO	OHO	AHO
Substrate		$S_{B,poly}$ or S_{VFA}	$S_{B,mono}$
Conditions of growth	ox, anox, ana	ox, anox, ana	ox
Rate of SB, mono storage into X_{STO} for AHOs, $q_{AHO,STO}$ (d^{-1})		–	6
Reduction factor for anoxic storage of AHOs, $\eta_{STO,AHO,anox}$			0.25
Reduction factor for anaerobic storage of AHOs, $\eta_{STO,AHO,ana}$			0.6
Maximum specific growth rate, μ_{Max} (d^{-1})	4	2	6
Half-saturation of readily biodegradable substrate, K_S ($g\ COD.m^{-3}$)	5	5	0.5
Half-saturation of O_2 , K_{O_2} ($g\ O_2.m^{-3}$)	0.05	0.05	0.5
Decay rate, b (d^{-1})	0.62	0.2	0.6
Yield ($g\ X_{BIO} \cdot g\ S_B^{-1}$)	0.67	0.67	0.6
N content of biomass (mg N/mg COD)	0.07	0.07	0.1
EPS content of X_{BIO} , $i_{EPS,XBIO}$ ($g\ COD.g\ COD^{-1}$)		0.11	
EPS content of X_E , $i_{EPS,XE}$ ($g\ COD.g\ COD^{-1}$)		0.01	
Half-saturation of O_2 for EPS, $K_{O_2,EPS}$ ($g\ O_2.m^{-3}$)		0.5	
Half-saturation of NO_3 for EPS, $K_{NO_3,EPS}$ ($g\ N.m^{-3}$)		0.1	
Half-saturation of NO_2 for EPS, $K_{NO_2,EPS}$ ($g\ N.m^{-3}$)		0.05	
Reduction factor for anoxic flocculation, $\eta_{EPS,anox}$ (-)		0.75	
Reduction factor for anaerobic flocculation, $\eta_{EPS,ana}$ (-)		0.5	
Rate of flocculation, q_{FLOC} (d^{-1})		70	
Arrhenius coefficient for flocculation, θ_{qFLOC}		1.1	
Fraction of colloidal substrate produced in biomass death, f_C ($g\ C.g\ X_{BIO}^{-1}$)		0.1	

ox: aerobic conditions; anox: anoxic conditions; ana: anaerobic conditions.

fractionation (Table 2), especially at low SRT. With a single set of parameters, the model captured the effect of SRT on EPS production, soluble and colloidal COD removal, while the base model (Sumo2) could not (light green lines on Figure 3(b) and 3(c)).

Effect of dissolved oxygen concentration

The DO level varied between 0.1 and 2 mg O_2/L for three different SRTs: 0.5, 1 and 1.5 d. The experiments on the DO effect allowed the calibration of half-saturation parameters

**Figure 2** | University of New Orleans (UNO) A-stage pilot plant configuration and flocculation factors ($\eta_{FLOC,Process}$) applied.

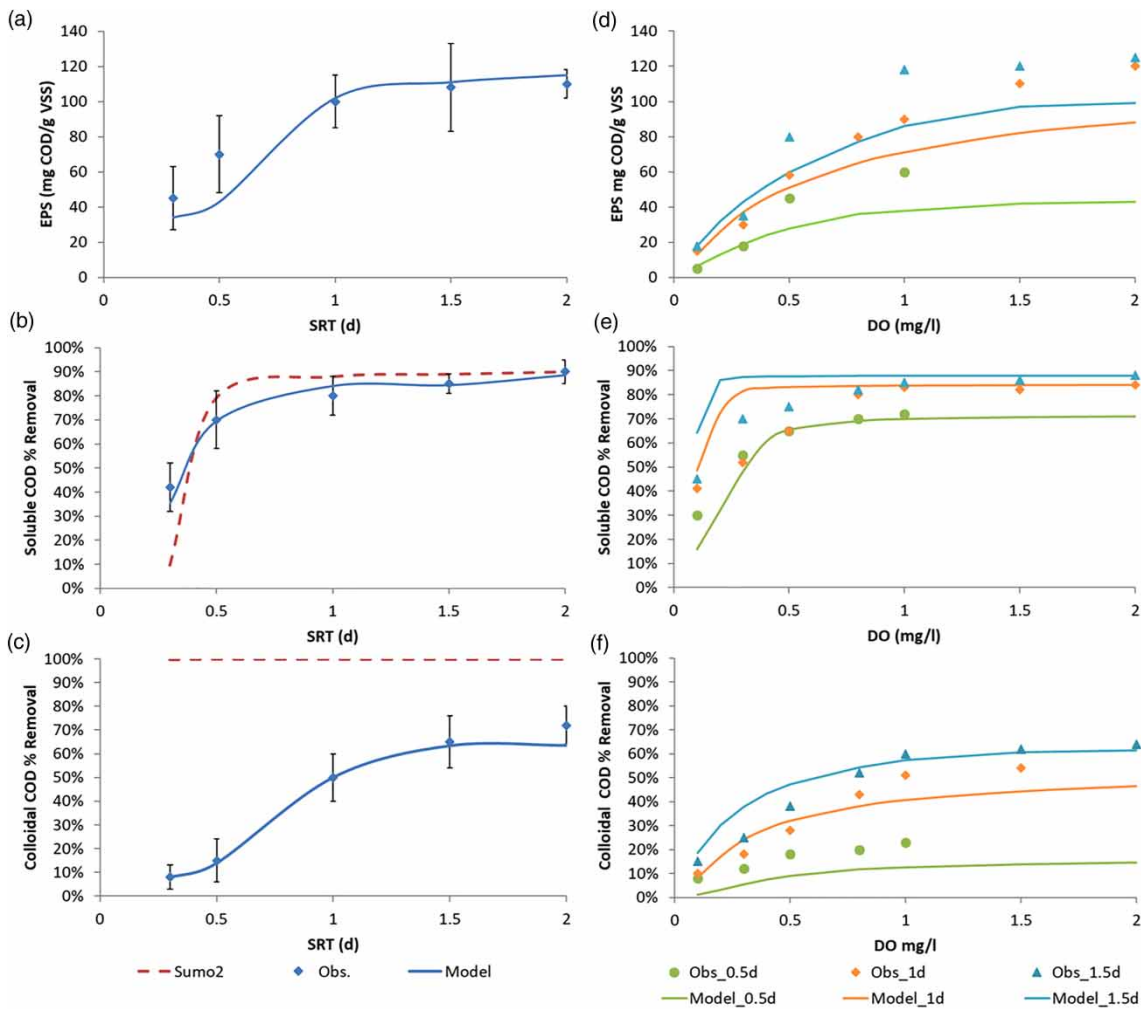


Figure 3 | Calibration results: SRT effect (a, b and c respectively for EPS, soluble COD and colloidal COD removal) and DO effect (d, e and f respectively for EPS, soluble COD and colloidal COD removal).

Table 2 | Influent characteristics of the two sets of experiments for the UNO pilot

Influent characteristics	SRT effect	DO effect
TSS [mg/L]	171	192
Total COD [mg COD/L]	395	457
Filtered COD [mg COD/L]	180	188
Flocculated filtered COD [mg COD/L]	120	119
Colloids [mg COD/L]	60	69
Fraction of heterotrophs (OHO) in total COD (TCOD) [%]	10	5
Influent carbon adsorption heterotrophs (AHO) fraction of the heterotrophs [%]	83	90
Readily biodegradable substrate as monomers (non-VFA) fraction of filtered COD [%]	75	80

for AHO growth and EPS calculation. All other parameters were kept at the values calibrated with SRT effect experiments. However, the influent characteristics and fractionation were slightly modified to better represent the quality of the influent at the time of the experiments (Table 2). It should be noted that this influent was fairly variable (Jimenez *et al.* 2015) and contains more particulate material than in the first set of the experiment. This may explain why the modelled EPS values are 33% lower than the observed ones (Figure 3(d)), as the $X_{\text{BIO}}/\text{VSS}$ ratio of the mixed liquor suspended solids (MLSS) is reduced (Equation (1)). Nevertheless, the effect of DO on EPS production is well captured by the model. The colloidal COD removal (Figure 3(f)) is well represented at 1 d and 1.5 d SRT, while at 0.5 d SRT the flocculation efficiency is more sensitive to the calculated EPS.

The soluble COD removal (Figure 3(e)) was closely predicted for 0.5 d SRT, while at lower DO the 1 d and 1.5 d SRT modelling results gave higher removal than observed. At these SRTs, the OHO population started to grow and out-competed the AHOs. A modification of OHOs parameters and especially an increase of the half saturation of O₂ and readily biodegradable substrate, would have resulted in better fit for this specific dataset. However, the objective was to create a valid model for the whole plant and overfitting to one dataset was avoided.

Overall, the model results were mostly sensitive to readily biodegradable substrate fractionation and influent biomass, as already noted by Nogaj *et al.* (2015) in their model.

Discussion on model calibration

The EPS measurement data using cation exchange resin (CER) extraction method developed by Frølund *et al.* (1996) is not specific to flocculent EPS. Three fractions of EPS may be defined: soluble EPS (also called soluble microbial product, SMP), loosely bound EPS (LB-EPS) and tightly bound EPS (TB-EPS), that can be fractionated with extraction methods (Li & Yang 2007; Kinyua *et al.* 2017). Tightly bound EPS will help to strengthen the flocs while loosely bound EPS (LB-EPS) will allow neighbour cell attachment. EPS are mainly composed of proteins and polysaccharides, proteins being more involved in the floc structure than polysaccharides (Dignac *et al.* 1998). Depending on operating parameters, the ratio of proteins/polysaccharides in EPS may change, which affects the bio-flocculation properties (Kinyua *et al.* 2017). However, Kinyua *et al.* (2017) show that not enough knowledge is available to understand the formation of EPS and the role of different EPS fractions in bioflocculation and floc structure. Therefore, the model presented in this study should be considered as a first step, including EPS formation and its role in bioflocculation. The model was developed to be simple for engineering use and general enough to be used to predict granulation. The model will evolve with new knowledge available in the future about EPS and bioflocculation.

Considering the EPS measurement method, the user may adapt the model calibration to their own range of measurement by adjusting the EPS content parameters (i_{EPS}) and the maximum flocculation rate (q_{FLOC}) to keep a similar order of flocculation kinetic rate value.

Based on the authors experience, the most sensitive parameters to be adjusted by the users are: (i) the flocculation reduction factor ($\eta_{FLOC,Process}$) that lumps all the

hydrodynamic effects affecting the shear force on the flocs (reactors geometry, type or aerators and mixers), this acts on the residual colloids; (ii) the influent characterization and especially the fraction of heterotrophs (OHO) in total COD and the influent carbon adsorption heterotrophs (AHO) fraction of the heterotrophs, that will be crucial at very low SRT to correctly predict the MLSS and the modeled EPS; and (iii) the readily biodegradable substrate as monomers ($S_{B,mono}$) fraction of filtered COD that will drive the residual rbCOD in the A-stage.

Model validation

Blue plains carbon-management pilot

The model was validated using a different set of data from a high rate pilot at Blue Plains Advanced Wastewater Treatment Plant, Washington, DC, USA. This pilot was chosen specifically because it represented a non-conventional high rate process to test the model ability to simulate carbon redirection and capture using the same mechanisms described in the model and calibrated for a conventional process. The detailed description of the Blue Plains Carbon Management pilot reactor operated at Blue Plains Advanced WWTP can be found in Rahman *et al.* (2016). The pilot was unique in that it represented a scenario of having a high rate system, with two configurations such as continuously stirred tank reactor (CSTR) and high-rate contact stabilization (CS), following a chemically enhanced primary treatment (CEPT). The wastewater characteristics were different than typical A-stage applications as the colloidal fraction was low due to the upstream CEPT process. Table 3 summarizes the average wastewater characteristics of the pilot feed (CEPT effluent).

Table 3 | Average wastewater characterization of blue plains carbon management pilot feed (CEPT effluent)

Parameter	Value
Total COD (tCOD) [mgCOD/L]	157
Particulate COD (pCOD) [mgCOD/L]	80
Colloidal COD (cCOD) [mgCOD/L]	22
Flocculated and filtered COD (sCOD) [mgCOD/L]	59
Total suspended solids (TSS) [mg/L]	31
Volatile suspended solids (VSS) [mg/L]	26
Ammonia [mg N/L]	23
Total phosphorus [mg P/L]	1.5
Ortho-phosphate [mg P/L]	0.8

The pilot reactor was run at a range of SRTs and two process configurations. The model was used to simulate a CSTR configuration and high rate CS configuration. To simulate the plug-flow nature of the pilot column, a series of four CSTR were used in the model to represent one pilot column. Table 4 summarizes the scenarios where the model was used for validation. Modifications to the flocculation reduction factor and $S_{B,mono}$ fractions were conducted to closely match the pilot effluent quality in terms of COD fractions. The flocculation reduction factors were increased to 75% for contactor column and 50% for the stabilizer. The increase was justified to account for the wall effects in the pilot columns that prevent good flocculation compared to full-scale tanks. The $S_{B,mono}$ fraction was changed to 60% for scenarios with temperatures above 20 °C and 40% for scenarios with 15 °C wastewater temperature. All other parameters were the same as these used in the model calibration (Table 1). Figure 4 summarizes the effluent quality for soluble COD (sCOD) and colloidal COD (cCOD)

Table 4 | Summary of blue plains carbon management pilot reactor's different scenarios used for model validation

Parameter	Unit	CS – 0.8 d	CS – 0.4 d	CSTR – 0.8 d	CSTR – 0.2 d
Stabilizer					
Volume	L	227	227	N/A	N/A
DO	mg/L	3.6	5.4	N/A	N/A
Contactor					
Volume	L	227	227	227	227
DO	mg/L	0.36	0.5	1.5	1.3
Total SRT	Day	1.4	0.7	1.2	0.3
Aerobic SRT	Day	0.8	0.4	0.8	0.2
Wastewater temperature	Celsius	27	22	15	27

N/A-not applicable, CS-contact stabilization, CSTR-continuously stirred tank reactor.

fractions for the pilot and the model predictions. In general, the model predicts the effluent quality for both process configurations quite well for the range of simulated SRT. The model was able to simulate the performance of colloidal capture of CS over CSTR by manipulating the flocculation coefficient, however, it also seems to be sensitive to SRT under the CS scenario where colloidal material capture under the short SRT CS scenario (0.4 d SRT) was not accurately predicted by the model.

MODEL APPLICATIONS

Rochester (MN) WWTP A-stage modelling

Rochester (MN, USA) WWTP A-stage (Figure 5) was modelled with the new model, without any parameter modification. The total SRT for the three tanks was 1.2 d. The flocculation factor in each tank has been adjusted: 0.15 for the aerated reactor, being mechanically mixed, 0.75 for the sludge blanket, which was considered as a separate tank. The RAS was returned through a screw pump, and a low increase in C_B/X_B and C_U/X_U ratio is used ($fr_{XB,CB} = 2$).

The simulation results are presented with measured data in Table 5. It shows that the new model, without any calibration of the parameters except the influent fractionation, matches the behaviour of Rochester WWTP A-stage systems.

AAA Rottenburg WWTP A-stage modelling

The AAA[®]-process (alternating activated adsorption; Wett *et al.* 2014) provides an alternating reactor arrangement with operation cycles involving an aeration-phase, a pre-settling phase, 50% simultaneous feeding phase into the sludge blanket and overflow discharge (at constant water level) and a phase for wasting of the settled solids directly

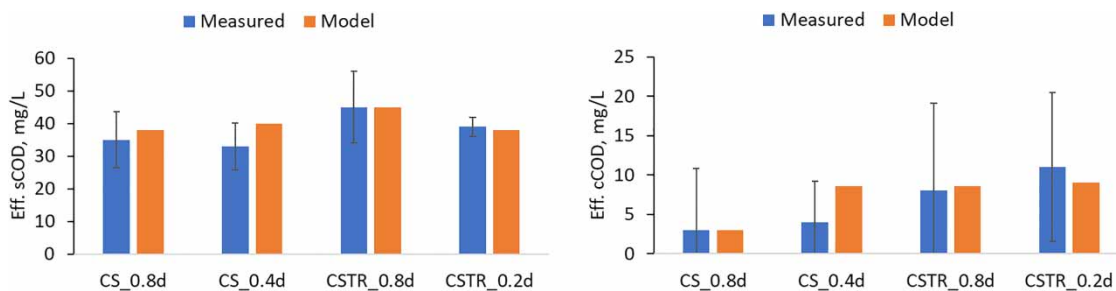


Figure 4 | Model validation against Blue Plains Carbon Management pilot performance for key parameters of effluent (Eff.) soluble COD (sCOD) and colloidal COD (cCOD) and associated standard deviations.

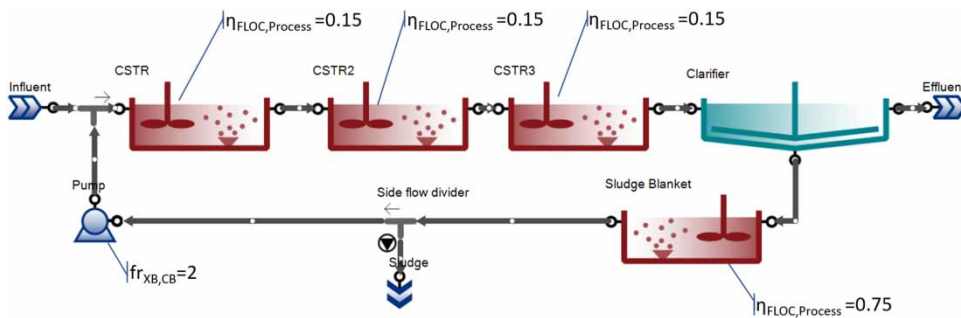


Figure 5 | Rochester (MN) WWTP A-stage configuration and flocculation factors ($\eta_{\text{FLOCC,Process}}$) and deflocculation fraction ($f_{r_{\text{XB,CB}}}$) applied for each process unit.

Table 5 | Comparison of Rochester (MN) WWTP A-stage system simulation results with measured data

	Influent	Effluent data (average of 10 d data)	Effluent model	Model error
TSS [mg/L]	66	94	94	
Filtered COD [mg COD/L]	229.1	67.2	61.3	-9%
Flocculated filtered COD [mg COD/L]	175	38.1	30.5	-20%
Colloids [mg COD/L]	54.1	29.7	31.9	6%
Total Kjeldahl nitrogen, TKN [mg N/L]	42	33.5	35.6	6%
Ammonia [mg N/L]	30	23.7	27	14%
Total phosphorus [mg P/L]	4	2.4	2.9	21%
Ortho-phosphates [mg P/L]	1.5	0.7	0.8	14%

to the adjacent thickener. The AAA-process is well suited for retrofitting existing rectangular primary clarifiers and requires an HRT of ca. 2 h. Half a year of data for winter-operation at the AAA-plant in Rottenburg (Germany), showed ca. two-thirds removal of the COD-load and one-third of the nitrogen load. From a modelling stand-point, this is an interesting case study of a system without any mechanical equipment and shear (flocculation factor of

0.9 for upflow sludge blanket) and a spatial discretization of an actually time-controlled process scheme (Figure 6). This way the model-configuration appears as a rather complex set-up of a reactive layered clarifier (upflow anoxic contactor) and a CSTR as an aerobic stabilizer, but the performance of the actually simple single-tank unit can be described very well (Table 6) without changing any stoichiometric or kinetic parameter of the model. The

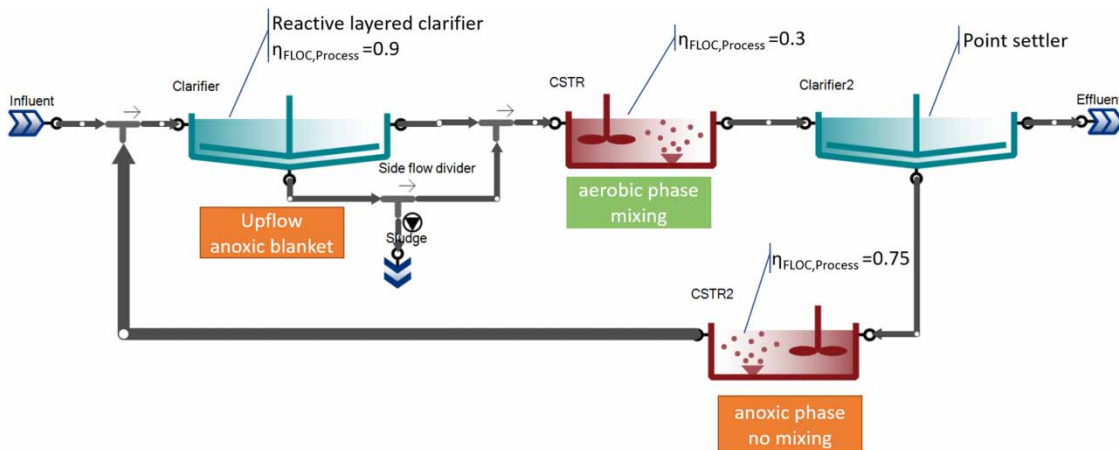


Figure 6 | AAA Rottenburg WWTP A-stage configuration and flocculation factors ($\eta_{\text{FLOCC,Process}}$) applied for each process unit.

Table 6 | Comparison of AAA Rottenburg WWTP A-stage simulation results with data

	Influent	Effluent data (2 month average)	Effluent model	Model error
Total COD [mg COD/L]	356	121	122	-0.8%
Filtered COD [mg COD/L]	152	83	84.6	1.9%
Total nitrogen [mg N/L]	43.3	30.2	29.8	-1.3%
MLSS [kg/m ³]		2.22	2.26	1.8%

modeled MLSS concentration is close to the observed MLSS and the nitrogen and COD removal are well described. The filtered COD contains both soluble and colloidal COD fractions. The model predicts 55% of filtered COD being colloidal, while a comparison with data is not possible due to missing flocculated filtered analysis.

CONCLUSIONS

A new model was developed to describe colloidal material removal and EPS generation, flocculation, and storage with the objective of extending the range of whole plant models to very short SRT systems, while maintaining existing and validated predictions in all other typical units of a WRRF. In this study, the model is tested against A-stage data and proved to match the COD and colloid removal at low SRT. The model was applicable for A-stage, AAA, CSTR and high-rate CS systems and was also tested on longer SRTs where effluents do not contain much residual colloids, and digestion where colloids from decay processes are present.

This new model is proposed as a new step towards a consensus model that should be able to fit the behaviour of colloidal material and biosorption in different types of configurations such as high-rate and low-rate systems including biofilm reactors (such as moving bed biofilm reactors, trickling filters) and anaerobic digesters.

SUPPLEMENTARY MATERIAL

The full Gujer matrix and parameters of the model can be downloaded at the following link: <http://www.dynamita.com/public/models/Sumo2C.xlsm>.

REFERENCES

- Dignac, M.-F., Urbain, V., Rybacki, D., Bruchet, A., Snidaro, D. & Scribe, P. 1998 [Chemical description of extracellular polymers: implication on activated sludge floc structure](#). *Water Sci. Technol.* **38** (8–9), 45–53. [https://doi.org/10.1016/S0273-1223\(98\)00676-3](https://doi.org/10.1016/S0273-1223(98)00676-3)
- Dold, P., Ekama, G. & Marais, G. 1980 A general model for the activated sludge process. *Progress in Water Technology* **12** (6), 47–77.
- Dynamita 2016 *Sumo User Manual*.
- Frølund, B., Palmgren, R., Keiding, K. & Nielsen, P. H. 1996 [Extraction of extracellular polymers from activated sludge using a cation exchange resin](#). *Water Res.* **30**, 1749–1758.
- Haider, S., Svardal, K., Vanrolleghem, P. A. & Kroiss, H. 2003 [The effect of low sludge age on wastewater fractionation \(S\(S\), S\(I\)\)](#). *Water Sci. Technol.* **47**, 203–209.
- Jimenez, J. A., La Motta, E. J. & Parker, D. S. 2005 Kinetics of removal of particulate chemical oxygen demand in the activated-sludge process. *Water Environ. Res. Res. Publ. Water Environ. Fed.* **77**, 437–446.
- Jimenez, J., Miller, M., Bott, C., Murthy, S., De Clippeleir, H. & Wett, B. 2015 [High-rate activated sludge system for carbon management – evaluation of crucial process mechanisms and design parameters](#). *Water Res.* **87**, 476–482.
- Kinyua, M. N., Elliott, M., Wett, B., Murthy, S., Chandran, K. & Bott, C. B. 2017 [The role of extracellular polymeric substances on carbon capture in a high rate activated sludge A-stage system](#). *Chem. Eng. J.* **322**, 428–434.
- La Motta, E., Jiménez, J., Parker, D. & McManis, K. 2003 Removal of particulate COD by bioflocculation in the activated sludge process. *WIT Transactions on Ecology and the Environment* **65**.
- Li, X. Y. & Yang, S. F. 2007 [Influence of loosely bound extracellular polymeric substances \(EPS\) on the flocculation, sedimentation and dewaterability of activated sludge](#). *Water Res.* **41**, 1022–1030.
- Nogaj, T., Randall, A., Jimenez, J., Takacs, I., Bott, C., Miller, M., Murthy, S. & Wett, B. 2015 [Modeling of organic substrate transformation in the high-rate activated sludge process](#). *Water Sci. Technol.* **71**, 971–979.
- Rahman, A., Meerburg, F. A., Ravadagundhi, S., Wett, B., Jimenez, J. A., Bott, C., Al-Omari, A., Riffat, R., Murthy, S. & De Clippeleir, H. 2016 [Bioflocculation management through high-rate contact-stabilization: a promising technology to recover organic carbon from low-strength wastewater](#). *Water Res.* **104**, 485–496.
- Rahman, A., Mosquera, M., Thomas, W., Jimenez, J. A., Bott, C., Wett, B., Al-Omari, A., Murthy, S., Riffat, R. & De Clippeleir, H. 2017 [Impact of aerobic famine and feast condition on extracellular polymeric substance production in high-rate contact stabilization systems](#). *Chem. Eng. J.* **328**, 74–86.
- Rahman, A., De Clippeleir, H., Thomas, W., Jimenez, J. A., Wett, B., Al-Omari, A., Murthy, S., Riffat, R. & Bott, C. 2019 [A-stage and high-rate contact-stabilization performance comparison](#)

- for carbon and nutrient redirection from high-strength municipal wastewater. *Chem. Eng. J.* **357**, 737–749.
- Sin, G., Guisasola, A., De Pauw, D. J., Baeza, J. A., Carrera, J. & Vanrolleghem, P. A. 2005 A new approach for modelling simultaneous storage and growth processes for activated sludge systems under aerobic conditions. *Biotechnology and Bioengineering* **92** (5), 600–613.
- Smitshuijzen, J., Pérez, J., Duin, O. & van Loosdrecht, M. C. 2016 A simple model to describe the performance of highly-loaded aerobic COD removal reactors. *Biochemical Engineering Journal* **112**, 94–102.
- Wett, B., Hell, M., Andersen, M., Wellym, Fukuzaki, Y., Aichinger, P., Jimenez, J., Takacs, I., Bott, C., Murthy, S., Cao, Y. & Tao, G. 2014 Operational and structural A-stage improvements for high-rate carbon removal. In: *IWA Specialist Conference – Global Challenges: Sustainable Wastewater Treatment and Resource Recovery*, Kathmandu, Nepal.

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