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Modelling of aerobic granular sludge reactors: the importance of hydrodynamic regimes, selective sludge removal and gradients

Nicolas Derlon[a,*], Mercedes Garcia Villodres[a,b], Róbert Kovács[c,d], Antoine Brison[a], Manuel Layer[a], Imre Takács[c] and Eberhard Morgenroth[a,e]

[a] Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf 8600, Switzerland
[b] WABAG Water Technology Ltd, Bürglistrasse 31, CH-8400 Winterthur, Switzerland
[c] Dynamita, 7 Eoupe, La Redoute, Nyons 26110, France
[d] Nonlineum, 37 Perjes str., Budapest 1165, Hungary
[e] ETH Zürich, Institute of Environmental Engineering, Zürich 8093, Switzerland
*Corresponding author. E-mail: nicolas.derlon@eawag.ch

ND, 0000-0003-4240-9827; AB, 0000-0003-3889-5105; ML, 0000-0002-8426-186X; EM, 0000-0002-1217-269X

ABSTRACT

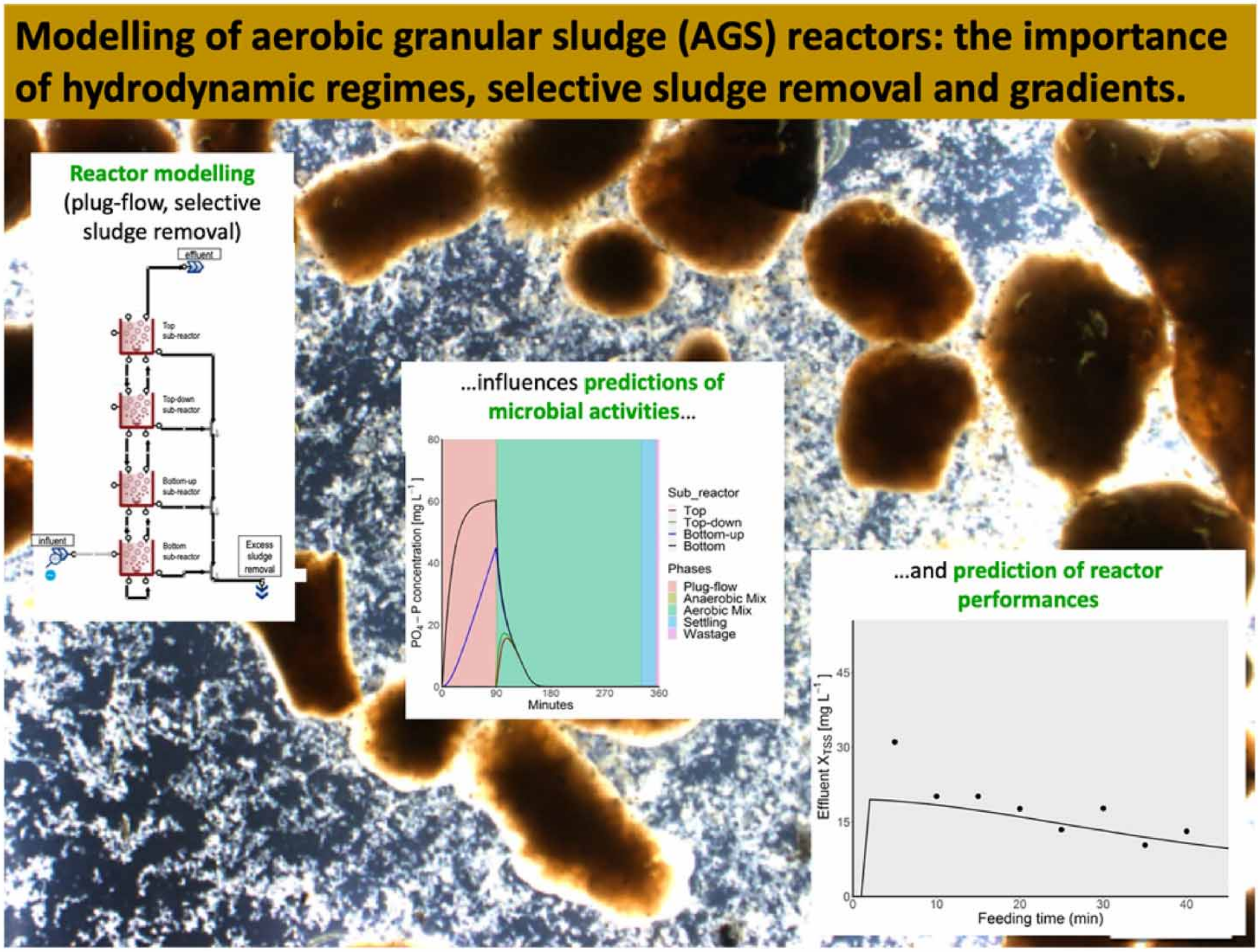
Hydraulic selection is a key feature of aerobic granular sludge (AGS) systems but existing aerobic granular sludge (AGS) models neglect those mechanisms: gradients over reactor height ($H_{reactor)}$, selective removal of slow settling sludge, etc. This study aimed at evaluating to what extent integration of those additional processes into AGS models is *needed, i.e.,* at demonstrating that model predictions (biomass inventory, microbial activities and effluent quality) are affected by such additional model complexity. We therefore developed a new AGS model that includes key features of full-scale AGS systems: fill-draw operation, selective sludge removal, distinct settling models for flocs/granules. We then compared predictions of our model to those of a fully mixed AGS model. Our results demonstrate that hydraulic selection can be predicted with an assembly of four continuous stirred tank reactors in series together with a correction code for plug-flow. Concentration gradients over the reactor height during settling/plug-flow feeding strongly impact the predictions of aerobic granular sludge models in terms of microbial selection, microbial activities and ultimately effluent quality. Hydraulic selection is a key to predict selection of storing microorganisms (phosphorus-accumulating organisms (PAO) and glycogen-accumulating organisms (GAO)) and in turn effluent quality in terms of total phosphorus, and for predicting effluent solid concentration and dynamic during plug-flow feeding.

Key words: aerobic granular sludge, gradients over reactor height, hydraulic selection, modelling, plug-flow feeding

HIGHLIGHTS

- New model for aerobic granular sludge system developed.
- Hydraulic selection of granules (bed stratification, plug flow feeding, etc.) are included.
- Gradients over reactor height predicted with a series of four CSTRs plus plug-flow correction code.
- Concentration gradients over $H_{reactor}$ strongly impact predictions in terms of microbial selection, microbial activities and effluent quality.

GRAPHICAL ABSTRACT



1. INTRODUCTION

Around 80 wastewater treatment plants based on aerobic granular sludge (AGS) and operated as sequencing batch reactors (SBR) are operational or under construction worldwide. However, AGS systems often experience long start-up phases (several months (Pronk *et al.* 2015b; Derlon *et al.* 2016)) or unsuccessful granulation. Also, the design and operation of AGS-SBR is mostly empirical, i.e., based on practical experience. Empirical design criteria are site/situation specific, while the results of dynamic models, when properly used, can be relied upon for generalizable accuracy (Rittmann *et al.* 2018). Dynamic models represent therefore a powerful tool for scientists, engineers, and practitioners. Models can be used by researchers to guide future research efforts and to better understand fundamental mechanisms. Models can also be used by engineers for the planning, design, optimisation, and evaluation of existing or new wastewater treatment plants (WWTP) (Boltz *et al.* 2010). But while the number of AGS systems implemented at full scale is growing rapidly, practicing engineers are still in need of a more appropriate AGS model.

1.1. Experiences from full-scale AGS-based WWTP and implication for model development

Full-scale AGS systems take advantage of both microbial and physical selection mechanisms to form granules. Several key features of AGS systems are still ignored in the structure of existing AGS models, while those mechanisms are of primary importance for granule formation and ultimately for the performances of AGS systems. We refer here to:

(1) the complex composition of AGS, characterized by the coexistence of flocs and granules,
(2) the existence of concentration gradients over the granule depth ($Z_{granule}$),

(3) the existence of concentration gradients over the reactor height ($H_{reactor}$) resulting from the plug-flow feeding and simultaneous fill-draw mode,
(4) the physical selection of granules using the feeding velocity and selective excess sludge removal of slow settling biomass or granules that are too large.

In the following sections we present some lessons learnt from our practical experience with full-scale AGS systems, and provide rationale for their consideration into AGS models.

1.1.1. AGS are hybrid sludge, with both flocs and granules

AGS always contain a small fraction of solids smaller than 200–250 μm[1], referred as 'flocs' in the current study (Pronk *et al.* 2015b; Derlon *et al.* 2016; van Dijk *et al.* 2018; Layer *et al.* 2019). The fraction of flocs in full-scale AGS plants usually varies between 0.1 and 0.2 (based on total suspended solid (TSS) measurements) (Figure 1) and comprises of granule debris, influent particles or biomass growing on organic substrate. AGS systems thus resemble hybrid systems, in which suspended biomass and biofilms coexist. The presence of flocs in AGS influences in turn the effluent quality, e.g., the effluent solids concentration (van Dijk *et al.* 2018). Flocs are also suspected to play an important role in capturing and converting the particulate organic substrates (Pronk *et al.* 2015b; Derlon *et al.* 2016; Campo *et al.* 2020; Layer *et al.* 2020a), thus having a key influence on the proper operation of AGS systems. However, most existing AGS models neglect their presence and in turn their contribution to the system performance (Beun *et al.* 2001; de Kreuk *et al.* 2007; Xavier *et al.* 2007; Ni & Yu 2010; Kagawa *et al.* 2015; Weissbrodt *et al.* 2017). We advocate the structure of AGS models should allow predicting the presence of floccular biomass to best predict the performances of AGS systems.

1.1.2. Gradients over the reactor height ($H_{reactor}$)

Another specific feature of AGS-SBRs is the formation of concentration gradients in both soluble/particulate compounds over the height of the reactor during the non-mixed phases (settling, anaerobic plug-flow feeding). Key for granulation is the selective uptake of substrates by the granules, which results from the stratification of the biomass bed during feeding. A representative bed stratification was characterized at the WWTP of Sarneraatal, Switzerland (Figure 2). Large granules (>2 mm) were found in the first 50 cm over the bottom (i.e., between 650 and 700 cm below surface), where they represented more than 90% of the biomass and reached a very high concentration (>30 gTSS/L). Smaller granules (0.25–2 mm) and flocs were equally observed between 50 and 450 cm above the reactor bottom at concentrations of 2.5–3 gTSS/L. The top of the

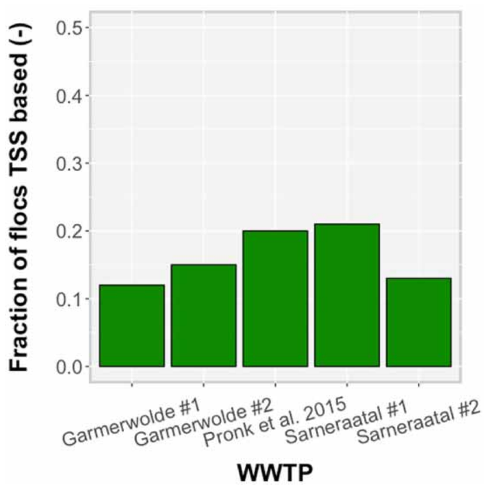


Figure 1 | Fraction of flocs (=solids smaller than 200–250 μm) (based on total suspended solid (TSS)) measured at different full-scale AGS plants.

[1] The cut-off between 'flocs' and 'granules' is arbitrary defined and different cut-off values are often reported in literature to make this distinction. However, typical values are usually ranging from 200–250 μm.

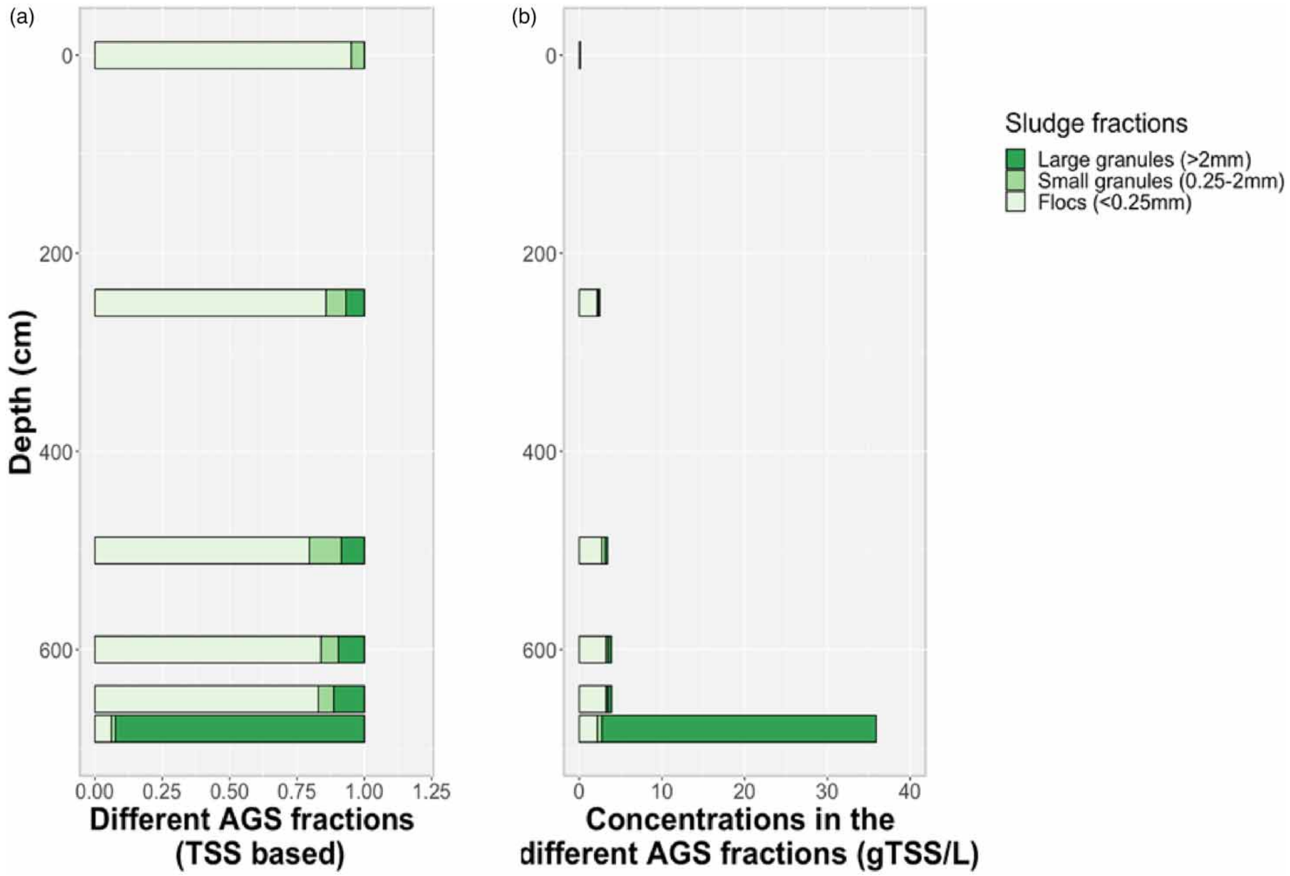


Figure 2 | Stratification of the sludge bed during non-mixed phase (here feeding) measured at the AGS plant of Sarneraatal, Switzerland. (a) different sludge fractions and (b) concentration of the different AGS fractions. 0 cm indicates the surface of the AGS reactor and 700 cm its bottom.

reactor consisted mostly of treated WW, therefore characterized by a very small solids concentration, below legal requirements (<20 mgTSS/L).

Those concentration gradients are essential to provide a competitive advantage to the granules. The distinct settling properties of the flocs and granules govern the stratification of the sludge bed. We advocate that the structure of AGS models (hydraulic reactor model, settling models for flocs and granules) should allow predicting concentration gradients over $H_{reactor}$.

1.1.3. Selective sludge removal

Selective sludge removal is applied at full-scale AGS systems to select granules over flocs (van Dijk *et al.* 2020) and to remove some particulate organic materials originating from the influent, e.g., cellulose (Pronk *et al.* 2015b). Selective sludge removal is usually performed at the top of the sludge bed after sedimentation or feeding, *i.e.*, at a certain depth and after a defined time. Slow settling flocs, small granules or granule debris are removed from the systems through this process (Pronk *et al.* 2015b; van Dijk *et al.* 2020). In some cases, sludge removal is also performed at the reactor bottom to remove large granules. Large granules have a small surface for mass-transfer, which limits their conversion rates. In existing AGS models, sludge removal is often 'forced' to reach an arbitrary fixed solid residence time (SRT) or to maintain granules only into the system. Instead, we suggest sludge removal in AGS reactor model should result from settling properties of sludge and location/time of the sludge withdrawal.

1.2. Limitations of existing aerobic granular sludge models

Many AGS models have been developed and are presented in Table 1. The development of these models clearly advanced our understanding of AGS systems, e.g., spatial distribution and interactions between microbial populations (Beun *et al.* 2001;

Table 1 | Overview of existing AGS models

References	Influent fractionation compatible with municipal WW	Microbial selection based on competition between storing and non-storing microorganisms	Hybrid biomass (flocs and granules)	Granule diameter(s)	Stratification over $z_{granule}$	Reactor volume (during feeding)	Liquid phase transport	Distinct settling model for flocs/granules	Stratification of the sludge bed	Selective sludge removal
Beun *et al.* (2001)	–	–	–	Fixed, one class-size	x	Variable	Continuous-stirred tank reactor (CSTR)	–	–	–
Su & Yu (2006)	x	–	x	Fixed, different class-sizes	x		CSTR	–	–	–
de Kreuk *et al.* (2007)	–	–	–	Fixed, one class-size	x	Variable	CSTR	–	–	–
Xavier *et al.* (2007)[a]	–	x	–		x	Variable	CSTR	–	–	–
Kagawa *et al.* (2015)[b]	x	x		Variable, different class-sizes	x	Variable	CSTR	–	–	x[c]
Ni (2013)		x	–	Fixed, different class-size	x	Variable				–
Su *et al.* (2013)	x	–	x	Variable, different class-sizes	x	Variable	CSTR	–[d]	x[e]	x
Weissbrodt *et al.* (2017)	–	–	–	Fixed, different class-sizes	x	Constant	Plug-flow and CSTR	–	–	–
Dold *et al.* (2018)	x	x	x	Variable, one class-size	x	Constant	Plug-flow and CSTR	–[f]	–[f]	x
Eawag AGS model (this study)	x	x	x	Fixed, one class-size	x	Constant	Plug-flow and CSTR	x	x	x

[a]Individual-based model.
[b]Individual-based model.
[c]Selective sludge removal during the 'reactor-scale model' period. Not clear how this selective removal was performed.
[d]Settling model for granules derived from layer model for secondary clarification.
[e]Stratification of the sludge bed predicted, but no plug flow feeding (6 min feeding followed by several hours aeration period).
[f]Only settling of the flocs is predicted. Granules are 'retained' in a bottom sub-reactor during feeding.

de Kreuk *et al.* 2007; Shinya *et al.* 2010), effect of dissolved oxygen (DO) on nitrogen removal (de Kreuk *et al.* 2007; Kagawa *et al.* 2015), etc. Most of these models are therefore able to predict the microbial selection of storing organisms (Lübken *et al.* 2005; Xavier *et al.* 2007; Ni & Yu 2010; Kagawa *et al.* 2015). But while hydraulic selection is also a key factor governing granules formation, only a few models are able to predict the coexistence of flocs/granules (Su & Yu 2006; Su *et al.* 2013; Dold *et al.* 2018), the plug-flow feeding (Weissbrodt *et al.* 2017; Dold *et al.* 2018), the stratification of the sludge bed (Su *et al.* 2013) or the selective removal of slow settling biomass (Su *et al.* 2013; Dold *et al.* 2018). Those aspects are, however, key features of AGS systems, as detailed in section 1.1. More importantly, none of them combine all aspects in link with hydraulic selection of granules, which limit their relevance for engineering practice (design, failure identification, system optimization).

1.3. Objectives

Our work thus aimed at developing an AGS reactor model that combines all aspects related to the microbial and hydraulic selection of granules, therefore correctly representative of the operation and functioning of full-scale AGS plants. A second objective of the work was therefore to demonstrate the importance of concentration gradients over $H_{reactor}$ on the model predictions (microbial population, prediction of effluent quality, etc.), in order to justify such increase in the complexity of AGS model. The goal was not to develop a fully calibrated AGS model validated on a full data set from an AGS-based WWTP. The 'Eawag AGS model' was implemented in Sumo© (Dynamita, Nyons, France) and consisted of a 1-D granule model, a reactor model (allowing for individual settling of granules and flocs and hence sludge bed stratification, plug flow feeding, selective sludge removal based on settling and removal at a specific location) and a bio-kinetic model. Simulations from the Eawag AGS model were compared to the simulations of a conventional fully mixed AGS model.

2. EAWAG AEROBIC GRANULAR SLUDGE MODEL

The Eawag AGS reactor model is an integrated model consisting of (1) a biokinetic model, (2) a granule model and (3) a reactor model. The AGS reactor model was implemented in Sumo® version 20 (Dynamita, Nyons, France) (http://www.dynamita.com). The model is available for download at: https://opendata.eawag.ch/dataset/eawag-ags-model-package. A full description of the model is provided in the package.

2.1. Biokinetic model

The Sumo1 biokinetic model was used in this study (Varga *et al.* 2018). This biokinetic model considers the following microbial populations: ordinary heterotrophic organisms (OHO), nitrifiers (NITO), phosphorus-accumulating organisms (PAO) and glycogen-accumulating organisms (GAO). The following microbial processes are included: (1) growth, (2) decay, (3) hydrolysis, (4) fermentation and (5) storage.

2.2. Granule model

A 1-D Granule model has been developed on the basis of the 'SumoBioFilm' Sumo® model. The 'SumoBioFilm' Sumo® model is a conventional 1-D biofilm model featuring a planar film surface. Our 1-D Granule model considers 2 distinct compartments, the bulk and the granules. The granule compartment is modelled as a sphere sub-divided into n layers (default value: $n = 6$). One main difference between the 1-D SumoBioFilm and the granule model is therefore the area of their layers. The area of the layers is constant over depth for the 'SumoBioFilm' model (planar surface), but variable over depth for the granule model (spherical surface). The diameter of the granules is fixed (input variable). The thickness of the four outer layers is fixed to 25 μm to increase resolution at the granule surface, while inner layers were distributed evenly depending on the chosen granule radius and the total number of layers (Layer *et al.* 2020b, 2022). The thickness of the inner layers is therefore calculated with the following equation:

$$Z_{inner,layer} = \frac{r_{granule} - n_{outer,layer} \cdot Z_{outer,layer}}{n_{total,layer} - n_{outer,layer}} \quad (1)$$

with $Z_{inner,layer}$ and $Z_{outer,layer}$ the thickness of the inner or outer layers (m), $r_{granule}$ the granule radius (m), and $n_{total,layer}$ and $n_{outer,layer}$ the total number of layer and the number of outer layers, respectively. The number of granules and therefore the overall granule volume is constant (input variable). Different mechanisms are considered in the 1-D granules model, using the same rate equations than the ones used in the 'SumoBioFilm' model: (1) attachment/detachment of particulate compounds, as governed by the concentration gradient between the bulk and top layer of the granules, (2) diffusion of soluble and colloidal compounds from the bulk into the granules and *vice versa*, with inclusion of a mass-transfer boundary layer (3) advection of particulate compounds between the granule layers (referred as transfer and displacement rates in Sumo®).

2.3. Reactor model

2.3.1. Overall structure

A main challenge was to develop a model structure allowing prediction of the stratification over the reactor height. A series of continuous stirred tank reactor (CSTR) can be used to create a pseudo two-dimensional (2-D) model of bulk-liquid hydrodynamics approaching plug flow (Boltz *et al.* 2017). The AGS reactor model thus consists of a series of four child-units assembled into an overall parent AGS reactor model (Figure 3). Each child-unit model is a modified version of Sumo's moving bed biofilm reactor (MBBR) model. This MBBR model represents a biofilm reactor operating at constant volume. The MBBR model was converted into a granules model (see section 2.2.) and additional hydraulic ports and connections were added to connect the four child-units together. Both water and soluble, colloidal and solid compounds (i.e., granules) can flow through those connections and therefore over the reactor height, allowing modelling of settling, granules wash-out with effluent, mixing conditions during mixed aerobic phase, etc. The reactor model additionally allows a variable volume, which is required when selective removal of sludge is applied. Moreover, the reactor model is equipped with an influent port (at the bottom) and an effluent port (at the top), thus allowing for operation in fill and draw mode.

2.3.2. Plug flow optimization

As our reactor model consists of a series of four CSTRs only, it only allows approaching plug-flow conditions. A correction code, active only during feeding, was therefore implemented to mimic an ideal plug-flow. The correction code helps

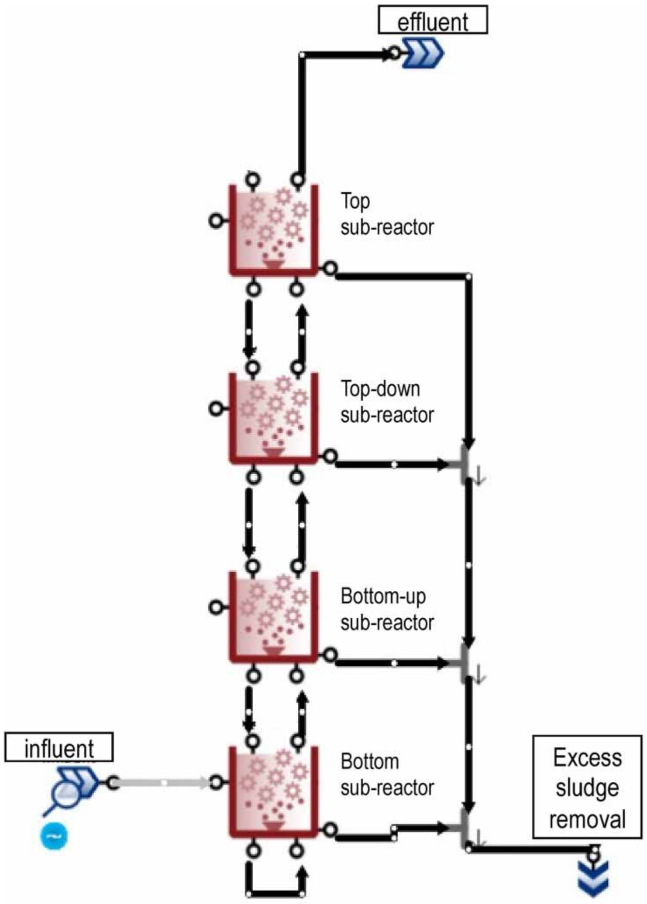


Figure 3 | Conceptual representation of the development of the AGS reactor model. Both water and soluble, colloidal and solid compounds (i.e., granules) can flow through the different connections and therefore over the reactor height.

'retaining' soluble compounds fed into a child-unit until the bulk volume has been fully exchanged. The bulk volume is calculated as the difference between the volume of a child-unit and the volume of granules.

2.3.3. Modelling sludge bed stratification

Stratification of the sludge bed is governed by (1) the settling properties of the granules and flocs, (2) the volume of the sub-reactors and (3) the feeding velocity ($v_{feeding}$). Settling of flocs into the pore space of the bottom child-unit is not possible. Also, the settling of granules (downwards) induces an upwards displacement of bulk (including flocs) towards the upper child-unit. Within each child-unit, the feeding velocity $v_{feeding}$ is calculated based on the available volume of the bulk compartment, i.e., the volume of interstitial voids in a child-unit where granules settled ($V_{reactor} - V_{granules}$) (Equation (2)).

$$v_{feeding} = \frac{Q_{inf}}{A_{reactor} \cdot \frac{V_{child-unit} - V_{granules}}{V_{child-unit}}} \tag{2}$$

where $v_{feeding}$ is the feeding velocity (m d^{-1}), Q_{inf} is the influent flow (m^3 d^{-1}), $A_{reactor}$ the reactor surface area (m^2), $V_{child\text{-}unit}$ the volume of the child-unit (m^3) and $V_{granules}$ the volume of granules contained in the child-unit (m^3).

An additional important aspect of the model is the volume of each CSTR that is adjusted by modifying the height of the sub-reactor, based on full-scale measurements and in order to reach an ideal stratification of the sludge bed: granules accumulated in the bottom sub-reactor only, for a voidage coefficient of 0.25 ($H_{bottom} = 0.57$ m), flocs in the bottom-up sub-reactor ($H_{bottom\text{-}up} = 3.64$ m), and the supernatant above in the top-down and top sub-reactors ($H_{top\text{-}down}$ and H_{top} of 2.1 and 0.7 m, respectively). Such adjustment of the sub-unit height/volume is directly derived from knowledge gained from full-scale plants and the cumulative height of the four sub-reactors, thus corresponds to the height of mixed liquor at the WWTP (here 7 m) (Figure 2).

2.3.4. Modelling sedimentation

Distinct models are implemented to predict independently the sedimentation of granules and flocs. The granule settling velocity ($v_{sett,gran}$, m/s) is calculated according to a discrete particle settling model, assuming spherical particles and following the Newton equations (MWH 2012). As can be seen from Equations (3)–(6), there is a circular dependency between the granule settling velocity and the Reynolds number. When implementing the model in Sumo, the tool recognizes these loops and solves them without manual interaction. The calculation of the granule settling velocity depends on the Reynolds number (Re).

$$Re = \frac{\rho_{H2O} \cdot 2 \cdot z_F \cdot v_{sett,gran}}{\eta_{H2O}} \tag{3}$$

If $Re < 2$ (laminar conditions) then:

$$v_{sett,gran} = \left(\frac{g \cdot (\rho_G - \rho_{H_2O}) \cdot (2 \cdot z_F)^2}{18 \cdot \eta_{H_2O}} \right) \tag{4}$$

If $2 < Re < 500$ (transient conditions) then:

$$v_{sett,gran} = \left(\frac{g \cdot (\rho_G - \rho_{H_2O}) \cdot (2 \cdot z_F)^{1.6}}{13.9 \cdot \rho_{H_2O}^{0.4} \cdot \eta_{H_2O}^{0.6}} \right)^{\frac{1}{1.4}} \tag{5}$$

If $Re > 500$ (turbulent conditions) then:

$$v_{sett,gran} = \left(\frac{4 \cdot g \cdot (\rho_G - \rho_{H_2O}) \cdot (2 \cdot z_F)}{3 \cdot c_D \cdot \eta_{H_2O}} \right)^{\frac{1}{2}} \tag{6}$$

where ρ_{H2O} and ρ_G are the water and granule density, respectively, z_F is the granule radius, η_{H2O} is the dynamic viscosity of water, g is the gravitational acceleration constant (9.81 m s^{-2}) and c_D the coefficient of drag (0.44 assuming smooth and rigid spheres). One may acknowledge that aerobic granules are not perfectly smooth and rigid spheres, and that the value of their drag coefficient might be larger than 0.44. However, the settling of aerobic granules mostly occurs under transient hydrodynamic conditions, for which the drag coefficient does not influence the settling velocity predicted by our model (Equation (5)). If the focus is on the prediction of the settling velocity under turbulent conditions, one would have to establish an empirical correlation between the Re number and the C_D coefficient of their granules (van Dijk *et al.* 2018).

The settling velocity of the flocs ($v_{sett,flocs}$, m/s) is calculated according to the Vesilind equation (stock Sumo settling model), which integrates floccular, hindered and compressed settling (Takács *et al.* 1991):

$$v_{sett,flocs} = \max(0; min(v_{max}; compr_{corr} \cdot v_{bnd} \cdot (e^{(-r_{hin} \cdot X_{TSS0})} - e^{(-r_{floc} \cdot X_{TSS0})}))) \tag{7}$$

where v_{max} and v_{bnd} are the maximum Vesilind and boundary settling velocity, respectively, r_{hin} and r_{floc} are the coefficients for hindered and floccular settling, respectively, and $X_{TSS,0}$ the effective X_{TSS} concentration in the bulk phase (max($X_{TSS,bulk}$-$X_{TSS,nonsettleable}$;0). $X_{TSS,nonsettleable}$ is an input variable. The compression term is calculated according to:

$$compr_{corr} = \min(1;\ e^{(r_{compr} \cdot (-X_{TSS,bulk} + compr_{on})})} \tag{8}$$

where r_{compr} is the coefficient for compression, $X_{TSS,bulk}$ the bulk X_{TSS} concentration and $compr_{on}$ the boundary compression concentration. One may however bear in mind that 'flocs' from AGS systems, i.e., all solids smaller than 250 μm, can contain a large fraction of dense debris resulting from granules breakage. The settling velocity of flocs from AGS systems might therefore exceeds the one of flocs from conventional activated sludge system.

2.3.5. Modelling of mixed conditions

During the mix phases of the SBR cycle (e.g., aerated phase), a very high Q_{mix} flow is applied between the different child-units to artificially create mixing conditions between the four child-units.

2.3.6. Excess sludge withdrawal

Each child-unit is equipped with a port for excess sludge withdrawal (Figure 3). Excess sludge withdrawal can occur through one or several ports. In the default Eawag AGS model, only flocs are withdrawn through excess sludge removal, but the removal of granules is in theory also possible if the model is used with a variable granules number/volume. Sludge wastage can be performed either selectively or based on a target SRT chosen by the user. Selective sludge withdrawal is governed by a combination of variables: settling velocities of the flocs and granules, duration of the sedimentation phase and depth of the port(s) selected for sludge extraction. In this case, a certain volume of bulk liquid is removed from a given sub-reactor, inducing a downward displacement of bulk liquid from the above sub-reactors (flow rates between sub-reactors computed according to the hydraulic balance). When excess sludge is withdrawn based on target SRT, the amount of wasted sludge is calculated according to the target SRT value, to the amount of solids lost with the effluent, and to the total amount of solids in the system. SRT calculation considers both the mass of flocs and of granules in the systems. However, only flocs are wasted (for both excess sludge removal modes). When only one port is used for excess sludge removal, the amount of sludge removed is limited by the amount of TSS in the bulk compartment of the corresponding child-unit. Sludge withdrawal can also be done via the removal of a certain bulk volume. In this case, the SRT is calculated according to the amount of solids withdrawn via excess sludge removal and via effluent.

2.3.7. Default scenario and parameters

Default parameters of the default scenario are listed in Table 2. Simulations were run for 150 d and data of one additional SBR cycle (0.25 d) was then extracted and analysed using R-Studio (Version 3.6.3, 2020).

2.4. Fully-mixed AGS model (reference model)

The fully-mixed AGS model consists of the same building blocks as the Eawag AGS model (a biofilm, biokinetic and reactor model). The granule/biofilm and the biokinetic model is similar to the one used in the Eawag AGS model. The reactor model consists, for the fully AGS model, of a single CSTR which is fully-mixed during all SBR phases and therefore operated in variable volume mode. No settling model is included as the sludge bed stratification is not predicted. Effluent total solids are an

Table 2 | Default SBR cycle parameters, biofilm model parameters and influent WW composition

SBR cycle parameters		Reference
Total cycle duration	6 h	Layer *et al.* (2020b), Layer *et al.* (2022)
Anaerobic feeding phase	Plug-flow, 1.5 h, up-flow velocity of WW during feeding $v_{ww} = 1.67$ m h^{-1}, settling granules/flocs ON	
Aerobic phase	Fully mixed, 4 h, constant dissolved oxygen (DO) concentration = 2.0 mg L^{-1}, settling processes are inactive during the aerobic phase	
Settling phase	Settling processes are active, 0.5 h	
Wasting phase	0.1 h, as part of the settling phase and selectively from second sub-reactor starting from the top of the reactor, to achieve a SRT_{target} = 20 d, settling processes are active during the wasting phase	
Volume-exchange-ratio (VER)	50%	
Hydraulic retention time (HRT)	12 h	
Biofilm model parameters		
Biofilm layers (n)	6	Layer *et al.* (2020b), Layer *et al.* (2022)
Granule radius (z_F)	750 µm	
Thickness of 4 outer granule layers (z_D)	0.25 µm	
Maximum granule X_{TSS} in the system ($X_{TSS,gran,max}$)	6.12 kgTSS $m_{reactor}^{-3}$	Layer *et al.* (2020b), Layer *et al.* (2022) SumoBioFilm model
Maximum X_{TSS} within the biofilm ($X_{TSS,max}$)	102 kgTSS $m_{compartment}^{-3}$	
Granule volume fraction ($X_{TSS,gran,max}/X_{TSS,max}$)	0.06 $m_{compartment}^{3}$ $m_{reactor}^{-3}$	
Influent composition	Value [unit]	SumoBiofilmModel
Total COD	420 mg L^{-1}	
Total Kjeldahl nitrogen (TKN)	34.4 mg L^{-1}	
Total phosphorus (TP)	4.3 mg L^{-1}	
Filtered COD fraction (incl. colloids, VFA)	40.5%	
Filtered flocculated COD fraction (incl. VFA)	20.2%	
VFA fraction of filtered COD	11.8%	
Unbiodegradable filtered COD fraction	11.8%	
Influent particulate inert COD fraction	14.0%	
Influent heterotrophic fraction of COD	5.0%	
Influent endogenous products fraction of OHOs	20.0%	
Unbiodegradable fraction of influent colloids	20.0%	
Ammonia fraction of TKN	69.8%	
Phosphate fraction of TP	58.1%	
N fraction of filtered biodegradable COD	4.0%	

(*Continued.*)

Table 2 | Continued

SBR cycle parameters		Reference
N fraction of unbiodegradable COD	1.0%	
P fraction of filtered biodegradable COD	1.0%	
P fraction of unbiodegradable COD	0.1%	

input parameter and are also not predicted. All details including a list of all parameters and default values of the fully-mixed AGS model can be found in Layer *et al.* (2020b, 2022).

2.5. Modelling scenarios

Different simulations were performed to highlight the importance of modelling gradients over $H_{reactor}$ on the prediction of the functioning and performances of AGS reactors (Table 3). Simulations were performed to assess (1) the modelling of the plug-flow feeding (scenario #1), (2) to evaluate the influence of concentration gradients over $H_{reactor}$ on the microbial selection and activities (scenario #2), and (3) to highlight the functionality of the Eawag AGS model to predict effluent quality or optimize operation of AGS-SBR (scenario #3).

3. RESULTS

3.1. Modelling plug-flow conditions (scenario #1)

A main attribute of the Eawag AGS model is to predict plug-flow hydrodynamic conditions during feeding (Figure 4). Plug-flow feeding predicted by our model was compared to predictions by a series of 10 CSTR and 100 CSTR (based on similar hydraulic retention time (HRT) of 1 d), using a non-reactive tracer (Figure 4). In the case of a series of 10 CSTR, breakthrough of tracer starts after 0.4 d only and 1.8 d are required to reach an equal substrate concentration in both the effluent and influent. A better plug-flow behaviour is predicted with a series of 100 CSTR: breakthrough starts after 0.8 d while the effluent trace concentration equals the influent concentration after 1.2 only. However, a perfect plug-flow feeding is predicted only by the Eawag AGS model (four CSTRs in series plus correction code). Breakthrough and equal tracer concentrations in influent and effluent are both observed at 1 d, corresponding to the HRT of the reactor.

Table 3 | Overview of the different simulation scenarios

Scenario	Main focus	Objective(s)	Models/conditions
Scenario #1	Modelling ideal plug-flow conditions during feeding	To evaluate the influence of combining CSTRs in series to model plug-flow conditions	10 CSTRs in series 100 CSTRs in series 4 CSTRs in series + correction code (Eawag AGS model) Non-reactive tracer.
Scenario #2	Impact of modelling concentration gradients over $H_{reactor}$	To demonstrate the importance of concentration gradient over $H_{reactor}$ for the prediction of population distribution, microbial activities and effluent quality.	Fully mixed AGS model: no gradient over $H_{reactor}$. Hydraulic selection is inactive. Eawag AGS model: gradients over $H_{reactor}$ are modelled. Plug-flow regime during settling and feeding (anaerobic) phases. Mixed conditions during the aerobic phase.
Scenario #3	Optimization of total nitrogen removal via optimized aeration	To highlight how the Eawag AGS model can be used to optimizing the operation and performances of AGS systems	Constant setpoint for aeration at 2 mgO_2/L Variable setpoint for aeration (first 2 mgO_2/L and then 0.5 mgO_2/L)

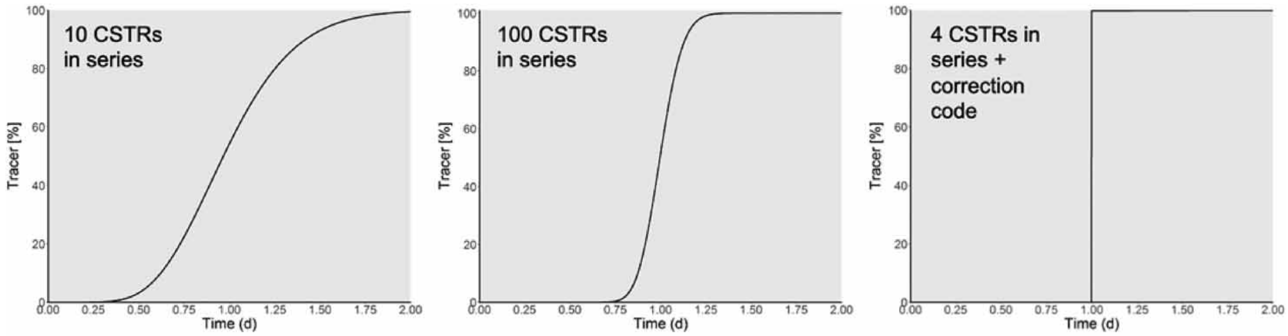


Figure 4 | Modelling of the plug-flow feeding with different model structures: 10 CSTRs in series, 100 CSTRs in series and 4 CSTRs in series plus correction code (as implemented in the Eawag AGS model).

3.2. Modelling of sludge bed stratification

Prediction of the distribution of flocs and granules in the four sub-reactors during the different phases of a default SBR cycle is shown in Figure 5. During the *settling and feeding phases (pink/blue phases)*, granules quickly settle towards the reactor bottom and accumulate exclusively in the bottom sub-reactor (black line), as the granule settling velocity always exceeds the feeding velocity in this default simulation. No granules are found in the upper sub-reactors. Flocs also settle during those *settling and feeding phases*. However, flocs mostly accumulate into the bottom-up sub-reactor, *i.e.*, on the top of the granules, and to a minor extent into the upper sub-reactor (top-down). Floc accumulation in the bottom sub-reactor is limited by the sedimentation of the granules, and the resulting upwards displacement of bulk volume. Floc concentration in the top sub-reactor mirrors the concentration of solids found in the effluent during feeding and is therefore very low. Overall, the sludge bed stratification predicted by the Eawag AGS model matches quite well the ones characterized at full-scale AGS-based plants, as the one of Sarneraatal WWTP shown in Figure 2.

During the mixed phases (green phase), the AGS reactor is then operated as a closed system (influent, effluent and wastage Q are nil) while a certain Q_{mix} flow is applied among the four sub-reactors to operate the AGS reactor consisting of four

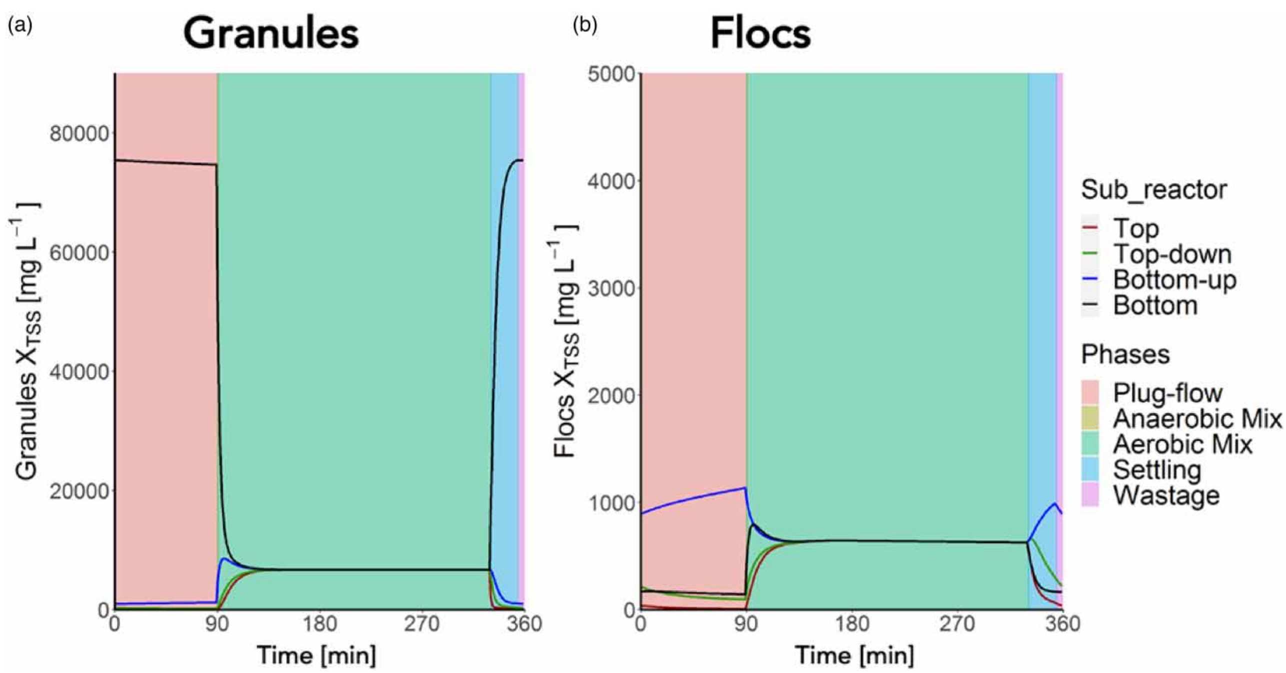


Figure 5 | Distribution of the (a) granules and (b) flocs over the different sub-reactors and different phases of the SBR.

CSTRs as a single CSTR. The flocs and granules concentrations thus equalize in each sub-reactor. During the *wastage phase (purple phase),* excess sludge withdrawal occurs in the top-down sub-reactor and only flocs are withdrawn.

3.3. How do concentration gradients over $H_{reactor}$ influence microbial activities and population distributions (scenario #2)?

3.3.1. Microbial activities

The influence of modelling stratification over $H_{reactor}$ was further investigated in terms of nutrient profiles (Figure 6) as a result of the different microbial activities (Figure 7).

Predictions by a conventional fully-mixed AGS model: during the mixed non-aerated feeding, nitrate concentration first decreases as a result of dilution and denitrification. Denitrification is taking place in the entire reactor volume due to mixed conditions. Once denitrification is completed and anaerobic conditions are established (t = 35 min.), the release of ortho-phosphates starts due to the activity of PAO and takes place until the end of the feeding phase (90 min). At t = 90 min, ortho-phosphate concentration in the bulk reaches a value of around 10 mgP/L. During the mixed aerobic phase, both nitrification by nitrifying organisms (NITO) and phosphorus uptake by PAO occur in parallel. Complete ammonium removal is achieved after 196 min (based on a legal requirement of 2 mgN/L), while full phosphorus uptake is predicted only after 208 min (legal requirement of 0.8 mgP/L).

Prediction by the Eawag AGS model (SCENARIO #2): the Eawag AGS model allows predicting the microbial activities over $H_{reactor}$ during feeding. An important PAO activity is predicted by the model, as shown by the significant increase in the ortho-phosphate concentration in the granule and floc bed (bottom and bottom-up sub-reactors, respectively). A complete release of ortho-phosphate by the granules accumulated in the bottom sub-reactor is also predicted after 50 min (Figure 6), as a result of the very rapid establishment of anaerobic conditions due to the quick denitrification taking place in the bottom sub-reactor (Figure 6). At the end of the feeding phase (t = 90 min), ortho-phosphate concentrations reach 60 and 45 mgP/L in the granule and floc bed, i.e., in the bottom and bottom-up sub-reactors, respectively (Figure 6, Eawag AGS model – ortho-phosphate profiles). This corresponds to a concentration of 20 mgP/L after a few minutes of mixing during the aerobic phase, as opposed to 10 mgP/L in the bulk predicted by the fully mixed AGS model. During the mixed aerobic phase, the uptake of ortho-phosphate by PAO is completed very rapidly after 156 min, as opposed to 208 min in the case of the conventional fully mixed AGS model. A similar observation is performed for the ammonium removal, which is also completed within 184 min by the Eawag AGS model, as opposed to 196 min predicted by fully mixed AGS model.

The differences observed in the nutrient profiles suggest modelling stratification over $H_{reactor}$ and plug-flow feeding influence in turn for the prediction of microbial activities (Figure 7). According to the fully mixed AGS model, the phosphate release rate (PRR) only starts to increase after 30 min of feeding once the nitrate uptake rate (NUR) is null, before reaching a constant rate of 10 mgP/L/h. In comparison, PRR starts directly with feeding and reaches a constant rate of 20 mgP/L/h when stratification/plug-flow feeding are predicted (Eawag AGS model). Similarly, the predicted phosphate uptake rate (PUR) is also strongly impacted by the model structure. A low PUR of max. 6 mgP/L/h is predicted by the fully mixed AGS model, as opposed to more than 30 mgP/L/h predicted by the Eawag AGS model. Comparable observations are possible regarding the ammonium and nitrate uptake rates (AUR and NUR, respectively), with slightly higher values predicted when stratification/plug-flow is considered in the model structure.

3.3.2. Implications for the microbial community composition

Modelling plug-flow feeding and sludge bed stratification has a major influence on the prediction of the sludge composition (flocs vs. granules) and on the microbial community composition (Figure 8). Fully mixed conditions favour the growth of OHO in the flocs and at the surface of granules (Figure 8). OHO growth predicted into the flocs and at the granules' surface by the fully mixed model exceed by 20 and 30% respectively predictions by the Eawag AGS model. The competitive OHO growth under fully mixed composition limits in turn the growth of PAO and GAO. The PAO + GAO concentrations are reduced by 13, 25, 25 and 11% in the layers #1–#4 of the granules of the fully mixed AGS model, as compared to the Eawag AGS model.

3.4. Functionalities of the Eawag AGS model (scenario #3)

3.4.1. Predicting system performances, e.g., effluent quality

An essential feature of the Eawag AGS model is its ability to predict the operation and performance of full-scale AGS plants. An example is given in Figure 9 for the dynamic of effluent solid concentration during bottom feeding with simultaneous

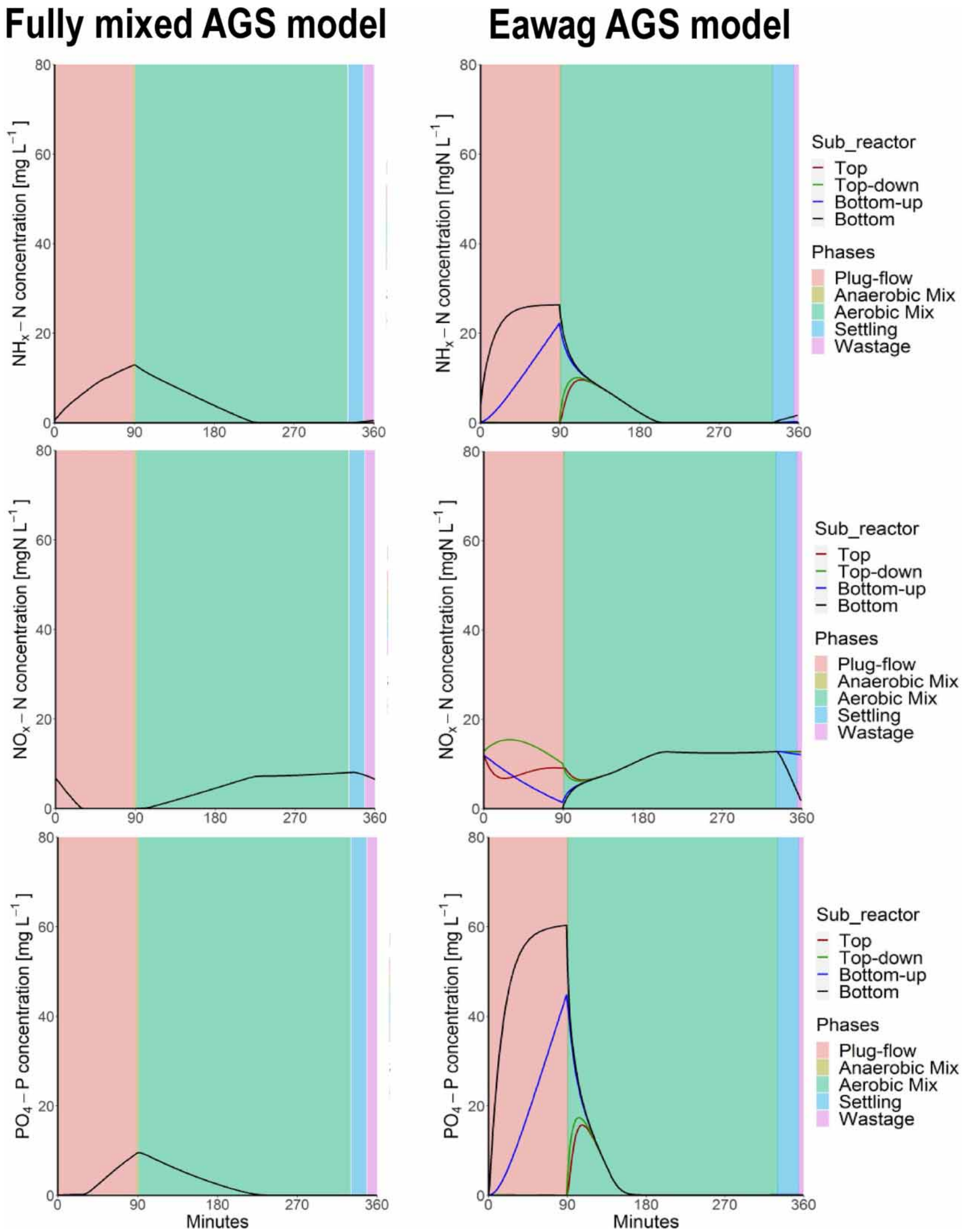


Figure 6 | Bulk concentration profiles of NH_x-N (top row), NO_x-N (intermediary row), and PO_4-P (bottom row) predicted by the fully mixed AGS model (left column) and Eawag AGS model (right column) over the different phases of the SBR cycle.

discharge of the treated wastewater at the top. Based on experimental data, the effluent solid concentration typically follows a decreasing trend during feeding, e.g., from 30 to less than 15 mgTSS/L after 40 min of feeding in the effluent. Such a decreasing trend is well predicted by our model with default settling parameters (no calibration). A gradual decrease of the effluent TSS concentration from around 20 mgTSS/L to less than 10 mgTSS/L at the end of the feeding is indeed predicted. Also, no leakage of ammonium from the influent into the effluent is predicted (perfect plug-flow, Figure 6). Ortho-phosphates are

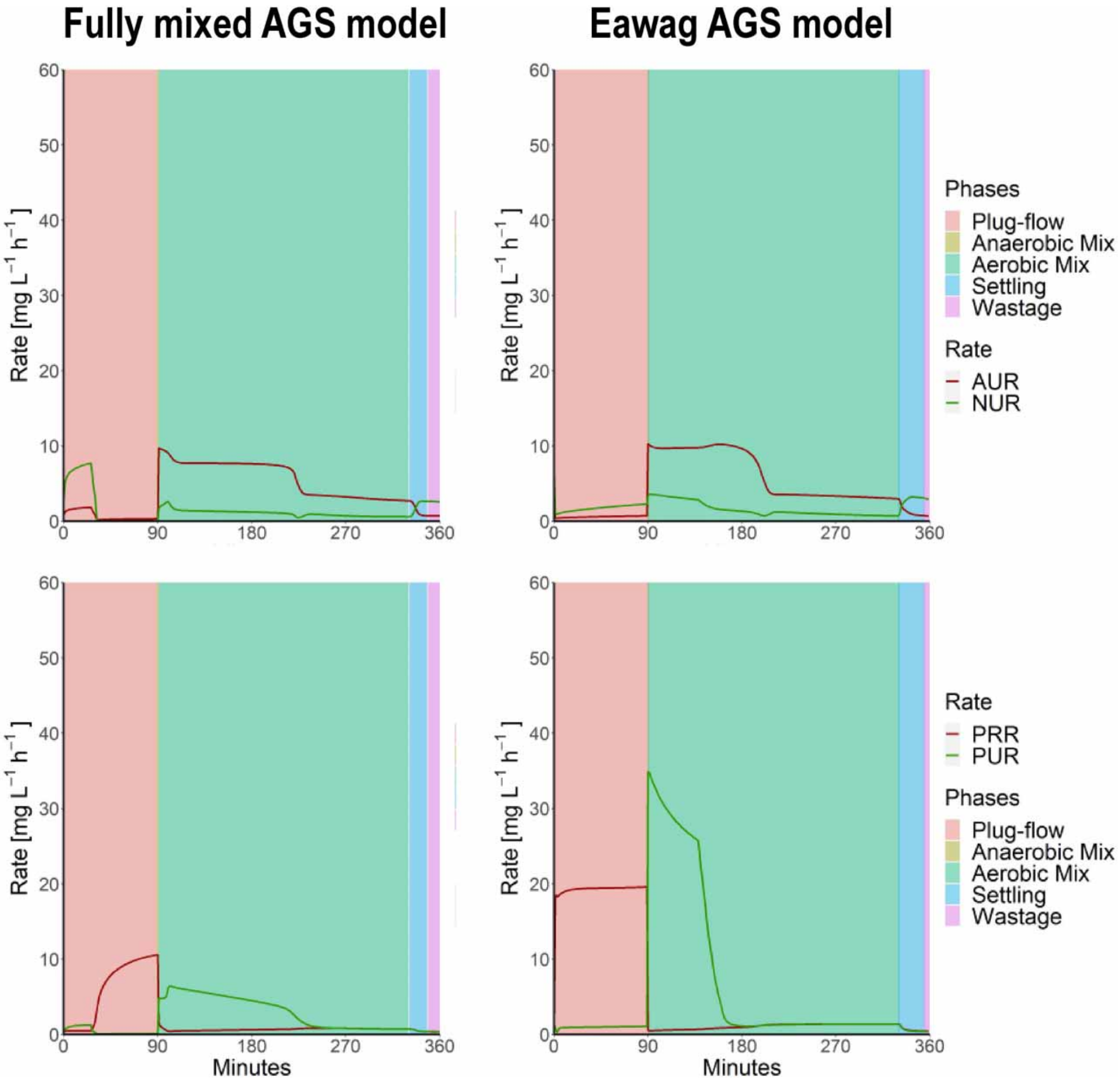


Figure 7 | Change in the nutrient conversion removal rates for the (a) conventional fully-mixed AGS model and for the (b) Eawag AGS model: ammonium uptake rate (AUR), NOx uptake rate (NUR), phosphate release rate (prr) and phosphate uptake rate (PUR).

released by both the granules in the bottom sub-reactor and the flocs in the bottom-up sub-reactor. The nitrate concentration follows a similar trend: with a slight decrease during the first half of the feeding followed by a slight increase and stabilisation during the second half.

3.4.2. Optimizing AGS-SBR operation using the Eawag AGS model

The Eawag AGS model also represents a tool to optimize the operation and performances of AGS systems, as for example the total nitrogen (TN) removal through smart aeration control (Figure 10). The Eawag AGS model allows predicting the penetration of oxygen over the depth of the granules (first row), the formation of the redox zone over the granule depth (middle row), and the resulting NOx concentration in the bulk (bottom row). At a dissolved oxygen set-point (DOSP) of 2 mgO_2/L in the bulk, granules are first partially penetrated by the oxygen, resulting in the formation of an aerobic zone at their surface while anoxic conditions prevail in their core (Figure 10, top left plot). Oxygen penetration gradually increased from 50 μm depth (90–140 min) to 100 μm depth (after 180 min). After 200 min, oxygen fully penetrates the granules, preventing the formation of anoxic conditions. Anoxic conditions thus form only for a short period in the core of the granule when a constant DOSP of 2 mgO_2/L is maintained (middle left plot), thus preventing denitrification and resulting in a rather large NOx accumulation in the bulk (bottom left plot).

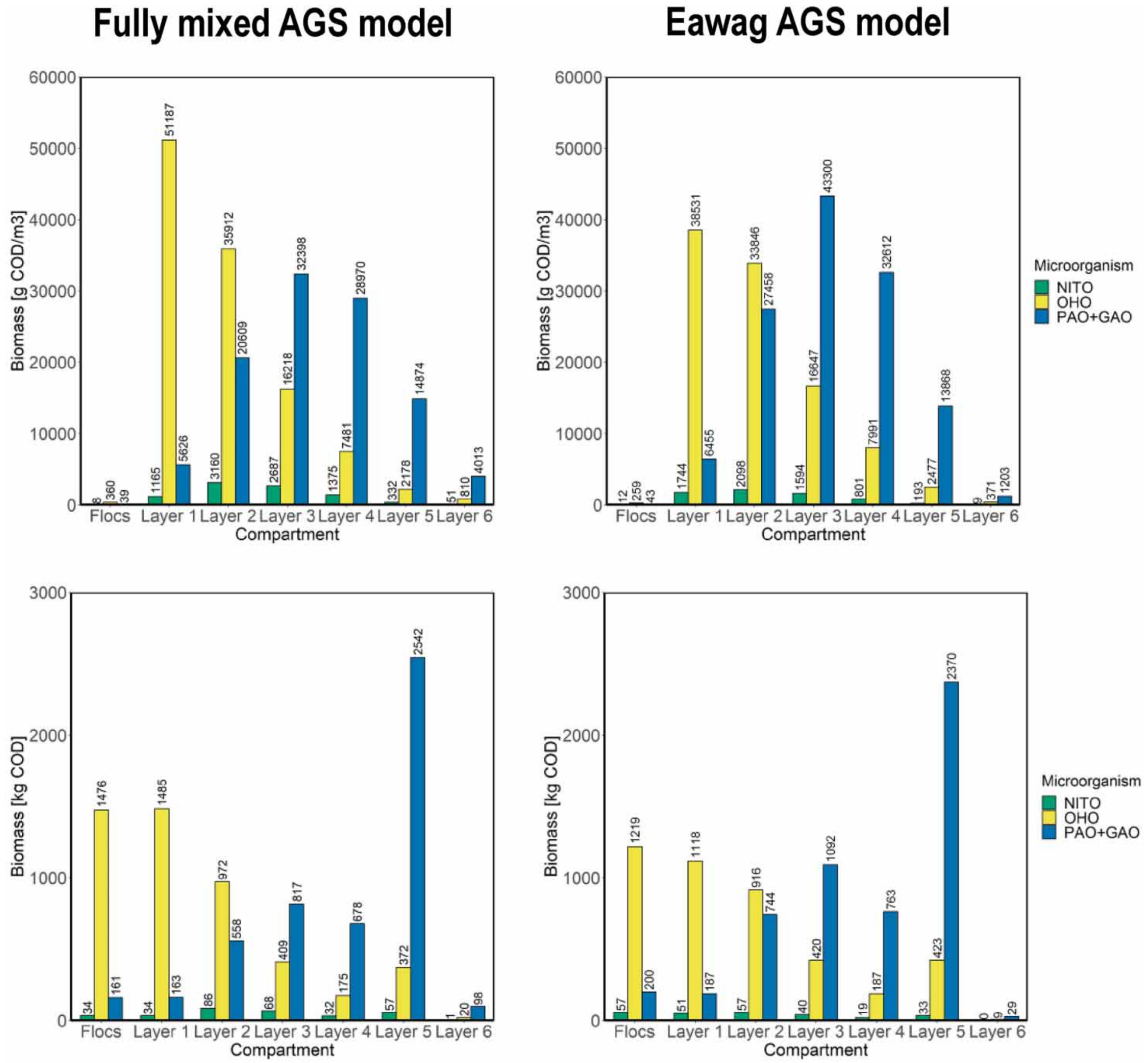


Figure 8 | Prediction of the microbial community composition within the flocs and granules, according to a conventional fully mixed AGS model (left column) vs. the Eawag AGS model (right column). Top row: biomass concentrations. Bottom row: biomass inventory.

The Eawag AGS model can be used by engineers to explore optimization strategies at a minimal cost/time, e.g., how to control aeration of their AGS-SBR to improve TN removal. In the example shown in Figure 10, a control of aeration at 2-DOSP (2 mgO_2/L for 30 min then 0.5 mgO_2/L) helped to better control the formation of the different redox zones and the utilisation of the organic substrate for denitrification (Figure 10, top right plot). As a consequence, and despite the complex composition of the influent (with a significant amount of non-diffusible electron donor), full nitrification-denitrification is predicted, resulting in a full TN removal (bottom right plot).

4. DISCUSSION

4.1. Gradients over $H_{reactor}$ matter: predict them!

Experimental evidence at laboratory and full-scale has long demonstrated that plug-flow feeding at the reactor bottom and selective removal of flocs is a key for the formation of granules. It is then intuitive to think that those processes should be

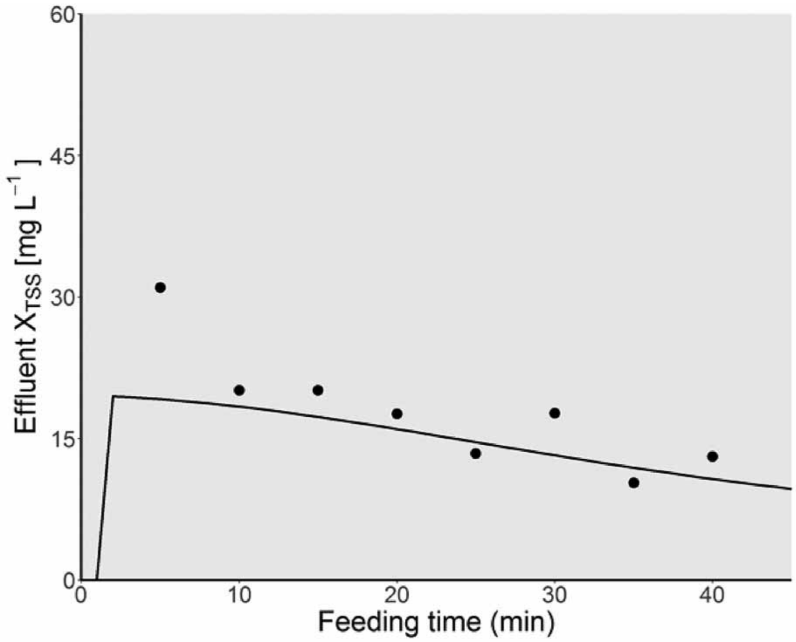


Figure 9 | Change in the TSS concentration in the effluent of AGS-SBR: experimental data from field test at Sarneraatal WWTP (black points) and predictions of the Eawag AGS model (black line).

incorporated into the structure of AGS models, while keeping the model structure 'as simple as possible, and as complex as needed' (Wanner *et al.* 2006). A first objective of our work was therefore to demonstrate that the integration of those processes into the structure of AGS models is *needed*. In other words, a key objective was to evaluate to what extent simulation results (biomass inventory, microbial activities and effluent quality) are affected by such additional model complexity. If model predictions are strongly impacted by plug-flow feeding/selective sludge removal and if those processes are essential features of the operation of full-scale AGS plant, it would then imply that those mechanisms must be considered in the structure of AGS models.

Our simulations confirm modelling gradients over $H_{reactor}$ does influence the prediction of microbial selection, and in turn the microbial activities and system performance (Figures 6–8). Modelling of the bed stratification and plug-flow feeding affects both the predictions of the biomass inventory and their spatial distribution over the granules radius. Fully mixed conditions during feeding favour accumulation of OHO, especially in the flocs and in the first layer of the granule (Figure 8). Ultimately, OHO and storing-organisms (PAO + GAO) were present in equal proportions within the granules (Figure 8). In contrast to this, modelling plug-flow feeding favoured accumulation of PAO + GAO, which in turn dominated the biomass inventory over OHO (Figure 8). Additionally, the concentrations of storing-organisms in the upper layers predicted by the Eawag AGS model exceeded the ones predicted by the fully-mixed model. The selection of slow growing microorganisms is a key for granulation and is enhanced during anaerobic feeding at the reactor bottom (de Kreuk & van Loosdrecht 2004; de Kreuk *et al.* 2005). The Eawag AGS model does not predict granule formation (constant total granule number/volume, one single size class) and is mostly dedicated to the modelling of plants with mature granules of steady diameter (Su *et al.* 2013). Yet, the competitive advantage predicted for PAO + GAO (inventory and spatial distribution) indirectly supports that granulation is favoured by a gradient over $H_{reactor}$, and that such processes must be predicted by AGS models.

As a result of the different spatial distribution and biomass inventories, microbial activities were also affected by the model structure, especially the biological phosphorus removal. The phosphate release rate predicted by the Eawag AGS model was twice as large as the one predicted by the fully mixed AGS model, while phosphate uptake rates were 5 times larger (Figure 7). As a consequence, ortho-phosphates were very quickly removed from the bulk during the aerated phase, as predicted by the Eawag AGS model. Our simulations were performed at a fixed SBR cycle duration (6 h total), and ultimately both models predicted full microbial conversion of substrates and nutrients. However, in practice, the length of the aerated phase is often controlled based on the ammonium bulk concentration. For example, the aerated phase is usually stopped once the

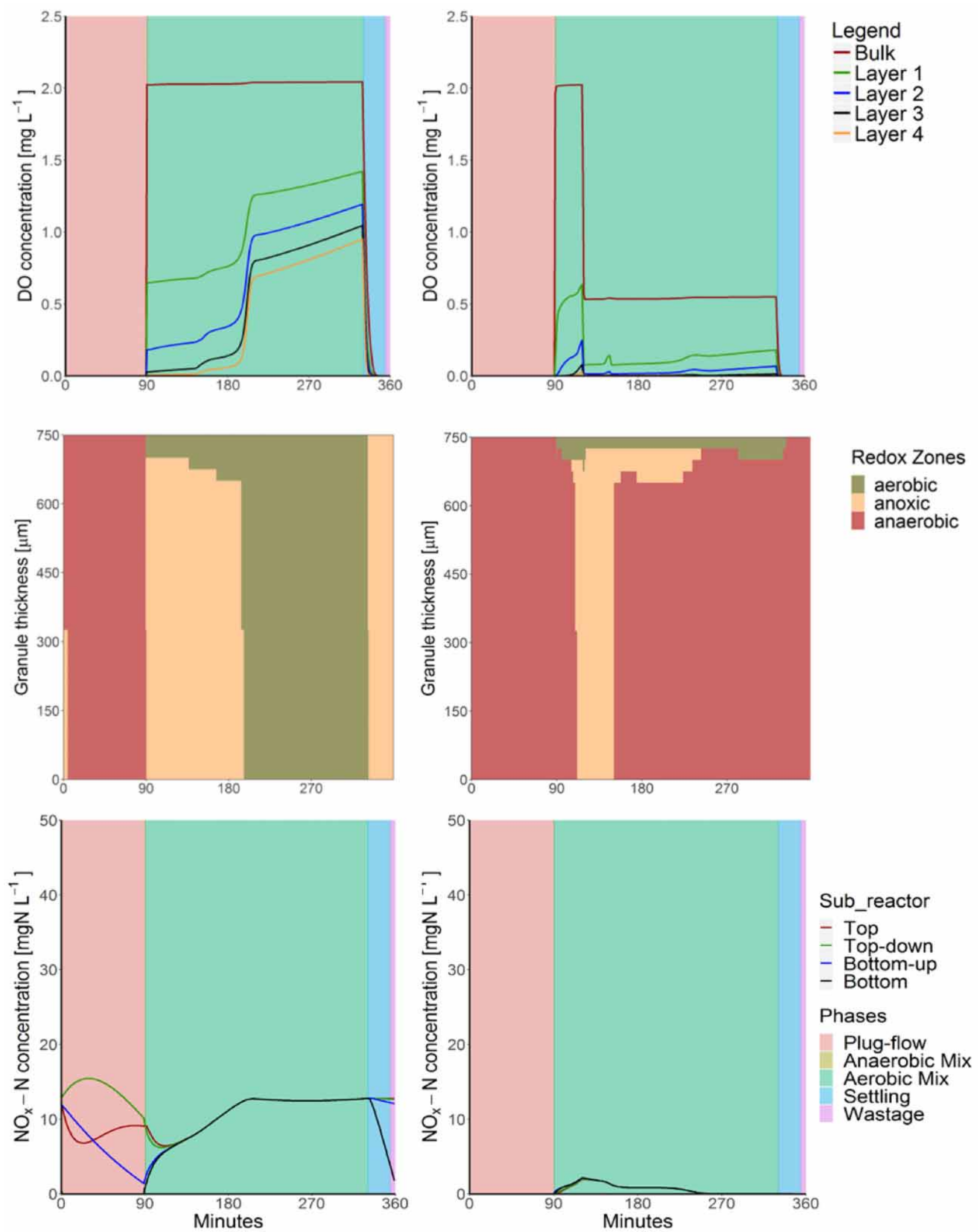


Figure 10 | optimization of the aeration control to improve total nitrogen removal (Scenario #3): aeration controlled at a constant dissolved oxygen set-point (DOSP) of 2 mg_{O2}/L in the bulk (left-hand column) as opposed to 2-DOSP (first 2 mg_{O2}/L and then 0.5 mg_{O2}/L) (right-hand column row). Plots show the dissolved oxygen (DO) concentrations in the different layers (top row), the resulting redox conditions developing within the granules (middle row) and the NOx concentrations (bottom row). The distinction between aerobic, anoxic and anaerobic redox conditions is based on the half-saturation constants of growth on O_2 and NOx of OHO of the Sumo1 biokinetic model.

ammonium concentration measured in the bulk reaches a threshold value lower than 2 mgN/L. Modelling of gradient over $H_{reactor}$ slightly affected the AUR predicted by both models and full ammonium removal was completed at almost the same time by the two models (208 vs 184 min for the fully mixed and Eawag AGS model, respectively). But prediction of the AUR is important to identify when the aerated phase should ideally be stopped. If aerated phase had been stopped once an ammonium concentration below 2 mgN/L was reached (Swiss legal requirement), the legal requirements on phosphorus would not be met according to the predictions of the fully mixed AGS model (e.g., PO_4^{3-} concentration of 1.4 mgP/L vs 0.8 mgP/L as requirement for TP). This is explained by the much lower PUR predicted by the fully mixed AGS model, due to the competitive advantage of OHO over PAO that resulted from the fully mixed feeding conditions. In addition to being inappropriate to predict granules formation based on microbial selection of PAO + GAO, fully mixed AGS models are also inept to model system performances and to optimize SBR operation. Despite that, our model was not calibrated, comparing its predictions to the ones of the fully-mixed AGS model clearly demonstrate the importance of integrating the hydraulic selection into the structure of AGS models.

4.2. How to model gradients over $H_{reactor}$?

The Eawag AGS model combines a reactor model with a 1-D granule model (see section 4.3 for the rationale of such a choice). A key question was therefore what is the best approach to model gradients over $H_{reactor}$.

Dold *et al.* (2018) combined a 1-D biofilm model with a 1-D layered solids flux model. The 1-D layered solids flux model is used to predict the settling of mixed liquor solids (non-granules) over n-layers of equal depth during settling, while the granules settle immediately at the reactor bottom at the beginning of the feeding (Dold *et al.* 2018). Conceptually, the overall reactor model used by Dold *et al.* (2018) thus consists of two child-units for a total of $n+1$ compartments: (1) a bottom child-unit containing the granules only and (2) a top sub-unit containing the supernatant with non-granule solids, divided in n-layers. An advantage of this approach is in offering a fine resolution for predicting gradients of growth conditions over the sludge bed, assuming a large n number is selected by the user.

In our model, gradients over $H_{reactor}$ are modelled using a series of four CSTRs combined with a correction code for plug-flow condition and using distinct settling models for flocs/granules. Our model thus resembles the model developed by Dold *et al.* (2018) with $n+1=4$ compartments. The number of compartments in our model implementation is fixed, and equals the number of CSTRs connected in series. Are four compartments sufficient to capture the behaviour of AGS systems, or do we need a finer resolution on the gradient above the granules bed? In our model, the depth of each compartment is 'set' by the user based on full-scale data to reproduce a representative sludge bed stratification, characterized by granules at the bottom, flocs on the top of the granules, and supernatant above (divided into two layers). Our model proved to be effective to predict the sludge bed stratification and in turn the effluent solids (both concentration and dynamic over feeding time) (Figure 9). It is then not evident that a finer resolution above the settled granule bed, as in the Dold *et al.* model, is required (as long as effluent quality and plug-flow conditions are well predicted).

Also, what counts when modelling full-scale AGS systems is what happens at the reactor bottom during settling/feeding, i.e., in the granule bed. The model developed by Dold *et al.* (2018) assumes that granules immediately form a settled bed under non-mixed conditions, i.e., that their settling at the reactor bottom is 'forced', thus consistently resulting in the formation of an ideal bed stratification. This is a major difference to our modelling approach. Our model is in fact predicting the settling of granules and flocs and thus the resulting sludge bed stratification. The predicted stratification of the sludge bed thus results from a balance between the settling properties of flocs/granules and the operating conditions (settling time, feeding flow). These processes can result in the formation of an ideal (only granules at the bottom receive substrate) or not so ideal sludge bed (granules are pushed in the second CSTR where they compete with flocs for substrate). One advantage of our model is that it allows the user to test different operating conditions (e.g., varying feeding velocities) to explore their effect on the sludge bed stratification and resulting microbial competition between storing- and ordinary heterotrophic biomass.

One may also argue that hydrodynamic conditions are not 'perfect' in a real AGS-SBR due to some upward/downward mixing during the anaerobic feeding. One may question to what extent representing 'perfect' plug-flow conditions is therefore necessary. But predicting a 'perfect' plug-flow feeding actually helps predicting a full-uptake of diffusible organic substrates by storing-microorganisms (Figure 8), as observed on full-scale AGS systems (Pronk *et al.* 2015a, 2015b). Such conditions are key for achieving a successful granulation. In this sense, it is therefore acceptable to predict perfect plug-flow conditions during the anaerobic feeding like with the Eawag AGS model.

4.3. To model or not to model concentrations gradients over $Z_{granules}$?

A core component of the Eawag AGS model is its 1-D biofilm model. A fair question is *why* a 1-D model, and *why not* a 0-D model for example? Diffusion limits transport of solutes inside granules and results in the formation of concentration gradients over its radius (de Kreuk *et al.* 2010). Gradients of growth conditions govern in turn the spatial distribution of the microbial populations and ultimately the system performances (de Kreuk *et al.* 2007). Operation of full-scale AGS systems in sequencing batch mode also implies solute concentrations in the bulk (and thus diffusion) vary significantly over the cycle length (Layer *et al.* 2020b). The longer the anoxic zone exists within the granules, the longer denitrification takes place and the higher the N-removal efficiency (de Kreuk *et al.* 2007; Layer *et al.* 2020b). While diffusion is key to the performances of biofilm systems and can be easily described mathematically, some AGS models do not incorporate this phenomenon directly. Instead, the limitation of microbial conversion rates by diffusion is lumped into the apparent half-saturation constant values (Lübken *et al.* 2005; Baeten *et al.* 2019). But as a first step, identification of apparent half-saturation constants actually requires knowing the spatial distribution of the microbial populations, and therefore using 1-D biofilm models (Baeten *et al.* 2019). Also, apparent half-saturation constants are sensitive to changes in the operating conditions (e.g., DOSP) as well as growth conditions (influent composition, temperature) (Baeten *et al.* 2019), while such long-term variations are typical of full-scale WWTP operation. Therefore, the use of 1-D biofilm models that predict directly diffusion and spatial re-arrangement of the microbial populations appears more appropriate. 1-D biofilm models were developed in the 1980s (Wanner & Gujer 1985, 1986) and are commonly used today in engineering practice for the modelling of biofilm reactors (Boltz *et al.* 2010). Guidelines on how to calibrate and apply a biofilm model are now available (Rittmann *et al.* 2018) to help users gaining accurate and meaningful results. The use of a 1-D biofilm model for the Eawag AGS model was therefore justified, with regards to the goals of the model.

5. CONCLUSIONS

- A stratified AGS model was developed to predict the performances of aerobic granular sludge systems. This new AGS reactor model includes key features of full-scale AGS systems: (1) simultaneous fill-draw mode operation, (2) selective sludge removal, (3) coexistence of flocs and granules, (4) distinct settling models for flocs and granules. It allows predicting concentration gradients over $H_{reactor}$ and $Z_{granules}$ during the different phases of the SBR operation, selective removal of slow-settling biomass, dynamic of effluent quality, etc.
- While most existing AGS models disregard gradients over $H_{reactor}$, we demonstrate predicting those gradients has a non-negligible effect on the predictions of AGS models. Concentration gradients over $H_{reactor}$ during settling/plug-flow feeding impact the predictions of microbial selection, resulting microbial activities and ultimately effluent quality.
- Concentration gradients over $H_{reactor}$ can be accurately predicted with a series of four CSTR combined with plug-flow correction code. The height/volume of each CSTR can be adjusted based on knowledge from full-scale AGS plants, to reproduce a representative sludge bed stratification during non-mixed conditions.
- The Eawag AGS model is a valuable tool for both science and engineering practice. The Eawag AGS model can be used by scientists to better understand fundamental mechanisms or identify possibly important research gaps. The Eawag AGS model can also be used by engineers for the planning, design, optimisation, and evaluation of existing or future AGS-based plants.

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DATA AVAILABILITY STATEMENT

All relevant data are available from an online repository or repositories: https://opendata.eawag.ch/dataset/eawag-ags-model-package.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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