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A dynamic compartmental model of a sequencing batch reactor (SBR) for biological phosphorus removal

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ABSTRACT

Bioreactors are usually modelled as continuous stirred tank reactors (CSTRs) or CSTRs connected in series (Tanks-In-Series configuration). In large systems with non-ideal mixing, such approaches do not sufficiently capture the complex hydrodynamics, leading to model inaccuracies due to the lumping of spatial gradients. Highly detailed computational fluid dynamics (CFD) models provide insight into complex hydrodynamics but are computationally too expensive for flow-sheet models and digital twin applications. A compartmental model (CM) can be a middle-ground by providing a more realistic representation of the hydrodynamics and still being computationally affordable. However, the hydrodynamics of a plant can be very different under varying flow conditions. Dynamic CMs can capture these changes in an elegant way. So far, the application of CMs has been limited mostly to continuous flow systems. In this study, a dynamic CM of a sequencing batch reactor (SBR) is developed for a bio-P removal process. The SBR comes with challenges for CM development due to its distinct operational stages. The dynamic CM shows significant improvements over the CSTR model (using the same biokinetic parameters) for dissolved oxygen and phosphate predictions reducing the need for model recalibration that can lead to over-fitting and limited extrapolation capability of the model.

Key words: biological phosphorus removal, compartmental modelling, computational fluid dynamics, sequencing batch reactors

HIGHLIGHTS

- CFD simulations showed incomplete mixing and stagnation zones in an SBR with an anaerobic/aerobic cycle.
- A dynamic compartmental model was developed for an SBR with an anaerobic/aerobic cycle.
- The impact of dynamic CM was investigated on biological phosphorus removal.
- The dynamic CM showed significant improvement in the model prediction power.
- CMs can reduce the calibration effort for the biokinetic models.

INTRODUCTION

Water resource recovery facility (WRRF) modelling is going through a transition from traditional process models to Digital Twin (DT) applications. A DT is a virtual replica of the physical system that simulates its operation in real-time and can be used for improved decision-making, predictive maintenance, online optimisation, etc. (Torfs *et al.* 2022). In order for a DT to remain reliable and robust over time, the predictive power of the underlying model is critical (Regmi *et al.* 2018). This will inevitably lead to a need for frequent model recalibration if the model predictive power is not sufficiently good enough (for the objective of the modelling study) or deviates from reality over time. A possible solution for this could be to use data-driven algorithms for automatic recalibration of the model parameters (de Almeida Martins *et al.* 2021). However,

this may not be the best practice if the discrepancies are related to flaws in the structure of the model. In the case of WRRFs, mechanistic models of the biological processes are the backbone of the DT. They are usually based on activated sludge models (ASMs) that have been developed to describe the biological carbon, nitrogen and phosphorus removal in wastewater treatment trains (Henze *et al.* 2006). Although there have been numerous studies on the calibration and validation of ASMs, the identifiability of most of their parameters remains a challenge (Sin *et al.* 2005; Sin & Al 2021). In addition, ASMs have been mainly benchmarked on municipal wastewater data (Gernaey *et al.* 2014). Industrial wastewater on the other hand shows highly variable characteristics which makes the application of ASMs an even more challenging task (Zhu *et al.* 2015; Monje *et al.* 2022). Consequently, a big effort usually goes into the calibration of the parameters of such models which can potentially lead to over-fitting problems due to the uncertainty of the parameters thus limiting their extrapolation capabilities.

Next to biological removal efficiency, the mixing and transport of carbon, nitrogen, phosphorous and oxygen components, play an important role in the performance of wastewater treatment plants. Wastewater treatment biokinetic models (i.e. ASMs) are usually implemented considering simple hydrodynamic representations such as a continuous stirred tank reactor (CSTR) or a number of CSTRs connected in series in the so-called Tanks-In-Series (TIS) configuration. TIS assume complete mixing inside the CSTRs and considers gradients in only one direction which is the direction of the flow (Levenspiel 1999). However, in many reactor configurations, this is far from the reality as more complex mixing leads to concentration gradients in different directions which can significantly impact the biological process (Rehman *et al.* 2017). Overly simplified hydraulic models lead to unnecessary calibration efforts for the biokinetic ASMs that can limit their predictive and extrapolation power (Gujer 2011). Hence, developing models with a more realistic representation of the system's hydrodynamics is becoming increasingly important when considering their real-time application for DTs, optimisation for more stringent effluent and energy requirements or real-time control purposes, all of which put high demands on the model's predictive power and require models to remain reliable and valid over a long time horizon. A model that fails to capture important dynamics of the system due to lumping spatial variations will not be able to achieve sufficient predictive power without cumbersome and not always reliable recalibration efforts.

Computational fluid dynamics (CFD) is used to model hydrodynamics with extremely high resolutions (in the order of centimetres) and has been shown to improve modeller's understanding of local mixing behaviour (Rehman 2016). However, CFD models are not widely used in the wastewater modelling community mainly due to them being computationally expensive. Alternatively, compartmental modelling (CM) represent a unique approach to model the hydrodynamics through a combination of functional zones, called compartments (Jourdan *et al.* 2019). These compartments, interconnected through exchange fluxes, can simulate the presence of dead zones or recirculation caused by non-ideal mixing. As such they are able to model concentration gradients in multiple directions making them much more powerful than TIS models without requiring the computational resources of a CFD model.

Local information about the gradients in the bioreactors is required to build a CM. This information could be obtained either from local measurements, expert knowledge or from CFD simulations, the latter being the most widely used. Some successful examples of CMs to model mixing behaviour in bioreactors can be found in the literature (Delafosse *et al.* 2014; Tajsoleiman *et al.* 2019; Massmann *et al.* 2020).

To build a CM from CFD models, the CFD simulations are mostly performed in steady-state and consequently provide only a snapshot of the bioreactor mixing patterns in time. However, the information about volumes and exchange flows between different regions can be used to build up the CM considering that they represent the most common operating condition of the system. The result is a fixed CM where the number of compartments, their volume and exchange flow between them is constant. This can be a reasonable assumption if the system is not highly dynamic and often represents a significant improvement compared to traditional TIS models. In case of having high variations in the local conditions due to for example extreme weather conditions or highly dynamic aerations, the assumption of fixed compartments and exchange flows will not hold and a dynamic CM would be more appropriate. In particular, non-continuous operations, like sequencing batch reactors (SBRs) are prone to highly dynamic local conditions. A dynamic CM can have different numbers of compartments, volumes and/or exchange flows depending on the dynamic operating conditions over time. However, building a dynamic CM usually requires several CFD simulations to cover a wide range of operating conditions in order to have a realistic representation of the real bioreactors.

Although there have been several studies on the CM for chemical reactors (Alexopoulos *et al.* 2002; Guha *et al.* 2006; Gresch *et al.* 2009; Vakili & Esfahany 2009), in the wastewater treatment domain, there are only a handful of applications

for CMs which mostly consider a continuous treatment process and a fixed CM configuration. While no previous study in the literature has been reported on the impact of hydrodynamics on the biokinetics of biological phosphorus removal, the effect of hydrodynamics on other biokinetic aspects has been proven to be significant. Le Moullec *et al.* (2010) conducted one of the first studies on the comparison of CFD, CM and the so-called systemic approaches where the flow is modelled through one reactor or some interconnected reactors like the TIS. The results showed a clear advantage of the CM compared to the TIS for dissolved oxygen (DO) and chemical oxygen demand (COD) concentration prediction in a conventional activated sludge system for carbon and nitrogen removal. Alvarado *et al.* (2012) did a similar study for a stabilisation pond where they extensively investigated the residence time distribution of different modelling approaches. The outcome was that the TIS (or in general the systemic approach) is not able to provide a good representation of the mixing patterns no matter the number and size of the CSTRs in the model and the further recalibration of the biokinetic model for solving a problem that is related to the structure of the model is not considered good modelling practice (Gresch *et al.* 2011; Gujer 2011; Le Moullec *et al.* 2011). Bellandi *et al.* (2019) did an extensive study on the comparison of TIS and CM for selecting the best model parameters that showed a narrower range of good values for the parameters thus improving the calibration effort and predictive power of the model. Most recently De Mulder (2019) and Borzooei *et al.* (2024) studied a CM approach for a full-scale treatment plant with enhanced biological phosphorus removal. Although the focus of those studies was on the implementation of CM for the aerobic and anoxic zones and therefore not on the biological phosphorus kinetics, the overall results show that the predictive power of the mechanistic biokinetic model was significantly improved for the DO and total suspended solids (TSS) concentrations. Nevertheless, all the previous studies showed the development of CMs for continuous systems and using a fixed CM configuration. The literature on the dynamic CM is even more limited. Some very recent studies showed the development of dynamic CMs (change in volume and exchange flows based on inlet flows of the bioreactors) for the fed-batch fermentation processes with improved results over the fixed CM approach in describing the local metabolic regimes in the bioreactor (Nadal-Rey *et al.* 2021; Bisgaard *et al.* 2022). De Mulder (2019) developed a dynamic CM for the aeration tank of a WRRF with adaptive volume/exchange flows based on the influent and air flow rate conditions. While it improved the predictive power of the model compared to the fixed CM, it needed several CFD simulations to cover a wide range of dynamics in the operating conditions of the continuous process.

Nevertheless, in all cases, CM shows promising improvements in model predictive power without further recalibration efforts for the underlying biokinetic model. This study presents a dynamic CM of an SBR for biological phosphorus removal of a maltery wastewater treatment plant. The SBR goes through different hydrodynamic phases due to the cyclic operation with and without aeration. This motivates the development of a dynamic CM which can adapt to different operating conditions based on the cycle time and therefore can demonstrate improved predictive power compared to the single-CSTR model.

METHODS

Case study

The bioreactor used in this study is a cylindrical sequencing batch reactor (SBR) treating maltery wastewater with the characteristic presented in Table 1. It has a volume of 5,200 m^3 and a depth of 6 m. The SBR cycle includes an anaerobic feeding phase (55 min) followed by an aerobic feeding phase (20 min) and a longer aerobic (non-feeding) phase (165 min) to provide optimal conditions for biological phosphorus removal. The effluent of the SBR goes to a membrane bioreactor which recycles

Table 1 | Characteristics of the maltery wastewater influent in the study

	Unit	Average value
COD	mg/L	2,587.4 ± 203
TN	mg/L	69.8 ± 9.9
TP	mg/L	22 ± 2.5
TSS	mg/L	364.2 ± 86.6
Q	m^3/d	2,009.2 ± 267.8

Note: The concentrations are mean values of nine samples in the month of March 2022. The flow rate is the mean daily value of the month of March 2022.

part of the wastewater back to the SBR. The aeration inside the SBR is controlled based on the DO concentration measured near the inlet of the SBR and using a combination of an on-off controller for activating the blowers and a PID controller to regulate the frequency of the blowers. The MLSS inside the SBR is kept at 9.5–10 g/L and the average sludge retention time (SRT) of the system is about 4.2 days. The waste-activated sludge is being removed from the SBR with an average flow rate of 170 m^3/d. Chemical dosing using iron chloride ($FeCl_3$) is done during the anaerobic phase to improve the phosphorus removal when the capacity of the biological phosphorus removal is not enough to remove all the phosphorus load coming into the plant during each cycle of the SBR (estimated based on lab-measured phosphorus uptake rate of 1.5 g P/kg VSS/hour). Overall, the plant shows 95, 97 and 94% of COD, TP and TN removal efficiency, respectively, over the 1 month period of the data presented in this study. Figure 1 shows the layout of the treatment plant.

High-frequency data were collected using the Oxymax COS61D sensor (Endress + Hauser, Switzerland) for DO and the Liquiline System CA80PH analyzer (Endress + Hauser, Switzerland) for phosphate (PO_4) to capture the dynamics of the phosphate release and update during the anaerobic and aerobic phases of the SBR cycle. These measurements were initially undertaken in different locations of the SBR to assess the homogeneity of mixing within the reactor. This exploratory step revealed variances in some parameters across different reactor zones, prompting the application of CFD to gain deeper insights into these mixing patterns.

In order to obtain the dynamics of the influent COD during the SBR cycles, high-frequency total organic carbon (TOC) data were collected at the influent wastewater using the TOCII CA72TOC analyzer (Endress + Hauser, Switzerland) and the optical TOC sensor Viomax CAS51D (Endress + Hauser, Switzerland). These measurements and laboratory COD data were analysed to establish a correlation between TOC and COD. This was an important step since readily biodegradable COD, which includes simple soluble substrates and volatile fatty acids (VFAs), is integral to the metabolic processes of phosphorus-accumulating organisms (PAOs).

Mechanistic biokinetic model

A mechanistic model of the treatment plant is developed in WEST (DHI, Denmark) simulation software using a single CSTR to describe hydraulics and the activated sludge model No. 2 (ASM2d) to describe biological phosphorus removal. It includes an aeration model (Rosso *et al.* 2005) to calculate the oxygen transfer rate based on the air flow rate supplied to the bioreactor. The controllers for the airflow based on DO concentrations are specifically implemented for this plant. This includes an on-off controller which activates three blowers based on different set-points of DO during different stages of

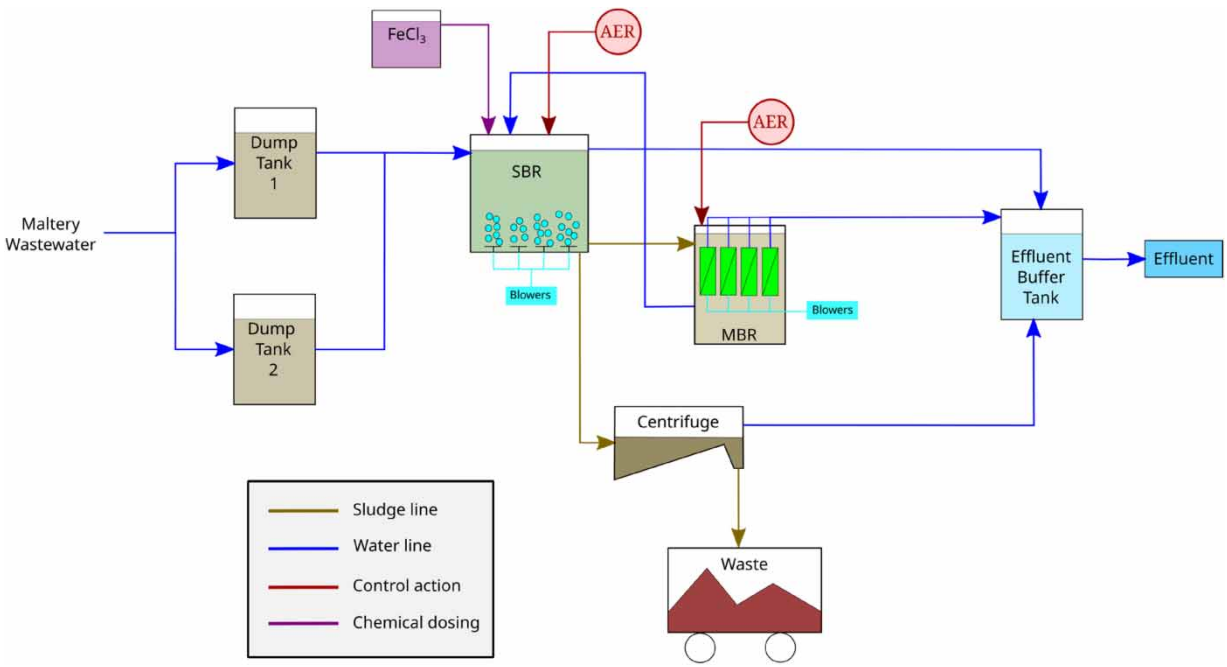

Figure 1 | Layout of the maltery treatment plant used in this study.

the SBR as well as a PID controller which regulates the frequency of the blowers during the second aeration phase (aeration without feeding). The model was calibrated and validated based on three weeks of dynamic data from the plant. The calibration was performed by changing the parameters one at a time and it followed the good modelling practice protocol (Rieger *et al.* 2012). The influent fractions were changed from the default values of the ASM2d model (Table 2). This was quite expected considering the difference in influent characteristics of the maltery wastewater compared to the conventional municipal one. Influent VFA and effluent COD lab measurement data were used for estimating the fraction of the fermentation product (F_S_A) and the fraction of soluble inert (F_S_I), respectively. While the model demonstrated satisfactory performance in simulating sludge balance and COD removal, with average relative errors of 3.7 and 4.6%, respectively, further calibration was necessary for the biological phosphorus removal parameters. This calibration aimed to fit the model's predictions more closely with the observed phosphate concentrations in the SBR bioreactor and effluent. The full list of the calibrated model parameters with their default values in the ASM2d model is given in Table 2.

CFD model

Although the mechanistic model performed well on average for the effluent quality, mixed liquor suspended solids, average DO and air flow rate, it lacked important dynamics of DO and showed an overestimation for the phosphate concentration. Considering the relatively big volume of the tank and the cyclic operation of the SBR with and without aeration phases, modelling the bioreactor as a single CSTR was considered a potentially important simplification. This was supported by a visual investigation of the bioreactor at the plant which showed inhomogeneous mixing patterns under different operating conditions. In addition, it is crucial for the model performance to have a good representation of the chemical dosing availability throughout the reactor to achieve good phosphorus removal predictions. Therefore, it was decided to investigate the mixing patterns inside the SBR by conducting a CFD study to investigate the mixing pattern which can impact the local concentration gradients. Three CFD simulations were done for anaerobic feeding, aerobic feeding and aerobic without feeding phases of the SBR cycle. The CFD model was built following the procedure reported in (Rehman 2016) with the geometry data of the bioreactor reported in Table 3. The meshing is performed using the commercial mesh/grid generator ICEM CFD, ANSYS with polyhedral mesh composed of a total of 3.3 million number of cells (Figure 2). Mesh independence test is performed starting with a coarser size until a fine mesh with sufficient performance is achieved. The mixture model is used for the multi-phase model. To reduce the computational demand of the simulations, only liquid and gas phases are considered in the multi-phase model in order to study the impact of aeration on the flow patterns. Besides, the solids are expected to have no significant impact on the aeration. The realisable k–ε turbulence model is used in this study. The mixers are modelled as momentum sources. Boundary conditions are defined based on the system knowledge. Inlet/outlet and air flows are

Table 2 | Calibrated influent fractions, kinetic and stoichiometric parameters of the mechanistic model

Parameter	Description	Calibrated value	Default value	Unit
Influent fractionations				
F_S_F	Fraction of fermentable readily biodegradable organic matter	0.5	0.375	–
F_S_A	Fraction of fermentation product (acetate)	0.45	0.25	–
F_S_I	Fraction soluble inert	0.05	0.375	–
F_X_S	Fraction of slowly biodegradable organic matter	0.1–0.3	0.69	–
F_X_H	Fraction of heterotrophic organisms	0.1	0.17	–
F_X_I	Fraction of particulate inert	0.6–0.8	0.14	–
Stoichhiometric parameters				
Y_PO4	Yield coefficient for phosphate release	0.26	0.4	gP/gCOD
Kinetic parameters				
Q_pp	Rate constant for storage of X_PP	2.5	1.5	1/d
b_PAO	Rate for lysis of X_PAO	0.1	0.2	1/d
Q_PAO_Stor	Rate constant for storage of PHA	1.2	3	1/d
b_PP	Rate constant for lysis of X_PP	0.03	0.2	1/d

Table 3 | The geometry data of the bioreactor used in the CFD model

Parameter	Value	Unit
Volume	5,200	m^3
Depth	6	m
Number of mixers	2	–
Mixers' diameter	2.5	m
Mixers' rotational speed	45	rpm

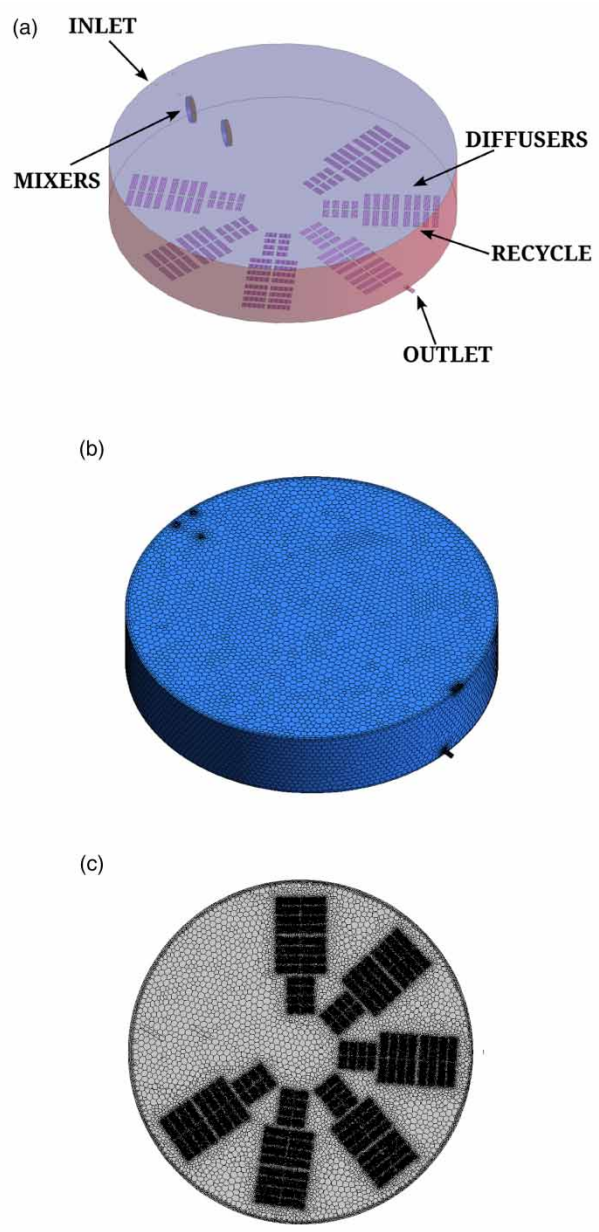

Figure 2 | (a) The scheme of the bioreactor geometry. (b) The meshing of the bioreactor. (c) The meshing around the diffusers at the bottom of the tank.

calculated based on known values while for the walls no-slip condition is considered (zero velocity at the walls). The symmetry boundary condition is used for the free surface on top of the reactor which is similar to the wall condition with zero wall friction. The $FeCL_3$ dosing was simulated as a tracer with transient simulations in order to investigate the required time for its complete dissolution in the reactor.

The CFD simulations are done in the Fluent, ANSYS commercial software using steady-state single-phase for the anaerobic phase and steady-state multi-phase for the two aeration phases of the SBR cycle. For investigating the dispersion of chemical dosing within the bioreactor, a transient simulation is performed for both anaerobic and aerobic phases to check which one is more optimal for the time of the dosing. For the aeration phases, an average air flow rate of 4,500 m^3/h is used based on the available data. Finally, the results of the CFD simulations are used to build a dynamic CM for the SBR which can switch between flow patterns of the anaerobic and aerobic phases.

RESULTS AND DISCUSSION

CFD model

The results of the CFD simulation in terms of the velocity vectors for the anaerobic phase are presented in Figure 3. A circular pattern can be seen inside the tank driven by the presence of the mixers. The inlet and outlet streams do not significantly affect the flow pattern inside the bioreactor. Interestingly, a stagnation zone is observed in the centre of the bioreactor (the region with the blue colours for the velocity vectors) which is almost cut-off from the main circular flow. Although the flow in both downward and upward directions are observed in that region, they are relatively very small compared to the rest of the tank with lower velocities towards the centre and bottom of the bioreactor.

Figure 4 shows the dispersion of $FeCl_3$ inside the bioreactor during the anaerobic phase after 10 min of the transient simulation. It is clearly visible that after this time the FeCl3 is not still homogeneously distributed in the reactor volume and it is much slower in the bottom and centre of the reactor. This can be explained by the presence of the stagnation zone in those areas. During the anaerobic phase, it takes almost 30 min for the chemicals to be distributed in the tank in a completely homogeneous way.

On the other hand, the results of the multi-phase CFD simulation during the first aeration phase of the SBR (Figure 5(a)) show a significantly reduced stagnation zone in the centre of the bioreactor due to the high air flow rates present in the tank. The impact of the aeration is much higher than the inlet flow rate (quite expected considering the difference in the flow rates; an average of 250 m^3/h for inflow compared to an average of 4,500 m^3/h for the airflow). As a result, the CFD simulation of both aeration phases (with and without feeding) is practically the same (data are shown only for aeration with feeding). Figure 5(b) shows the air volume fraction during the aeration phase. The distribution of the air within the bioreactor is highly affected by the circular and vertical flow driven by the mixers. In general, the air is less present in the areas where

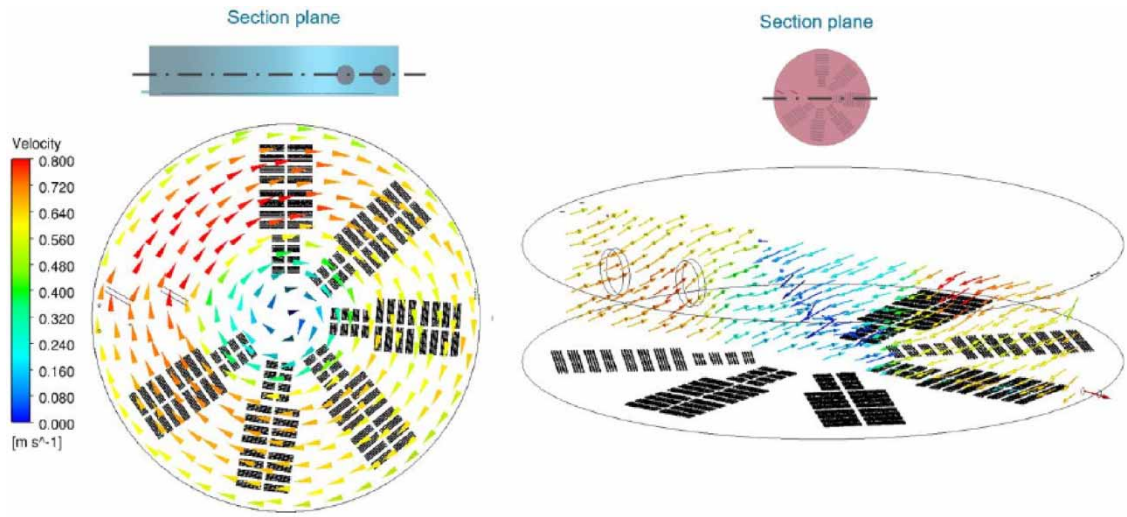

Figure 3 | The velocity vectors simulated with the CFD model for the anaerobic phase of the SBR.

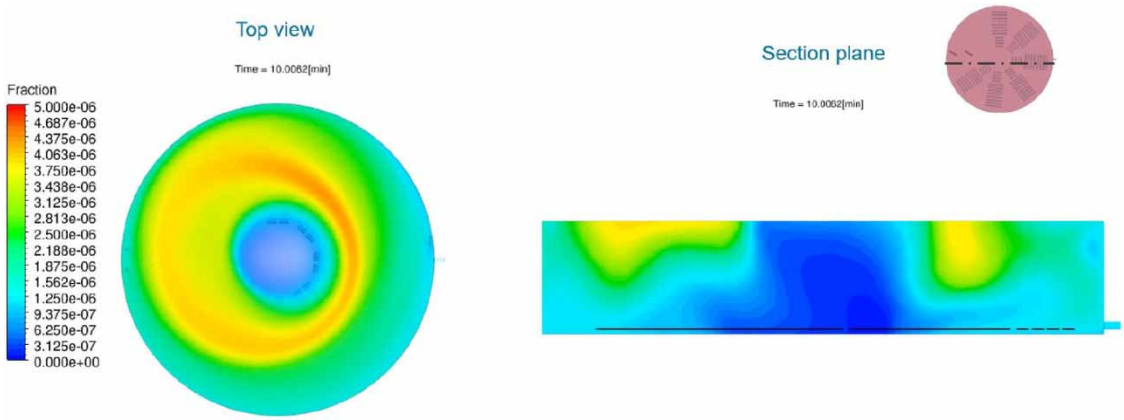

Figure 4 | The result of the transient CFD simulation for the dispersion of $FeCl_3$ in the bioreactor injected during the anaerobic phase at time = 10 min after the start of simulation.

there are no diffusers. The centre of the tank (the stagnation zone during the anaerobic phase) shows much less air compared to the rest of the tank. This is more visible when comparing the air volume fraction at different depths of the bioreactor (Figure 5(c)).

The dispersion of the $FeCl_3$ during the aeration phase is much faster compared to the anaerobic phase. In fact, after only 3 min of the transient simulation time (Figure 6), the chemical is already distributed quite well within the bioreactor. In this case, the total dispersion is achieved after almost 8 min compared to 30 min during the anaerobic time. Based on this, it is a wiser choice to add the chemical during the aeration phase instead of the anaerobic one in order to achieve a better phosphorus removal performance.

Dynamic CM

Based on the observations from the CFD simulations, it was decided to derive a compartment model to better capture the mixing dynamics in the SBR. The number of compartments, the volumes of the compartments and the exchange flows between them are then calculated from the CFD data. The compartmentalisation procedure is the same for both anaerobic and aerobic phases and it follows the step-wise approach presented in Rehman (2016). Thresholds to decide on the number of compartments are defined based on the variations in the velocity vectors and air volume fractions observed in different regions of the bioreactor. The idea is to represent the heterogeneity of the flow patterns as accurately as possible but with the smallest number of compartments possible to avoid high complexity and computational cost for the model simulation. In this study, it was observed that the flow patterns can be first divided in the direction of the convective flow in two main regions separating the part of the bioreactor where the air diffusers are located. This seems to be a reasonable assumption considering the air is mostly distributed in that region along the vertical axis with the rest of the bioreactor without diffusers showing an air volume fraction of mostly between 0 and 0.007 compared to values up to 0.015 above the diffusers. In addition, it was decided to create a compartment for the stagnation zone observed during the anaerobic phase. This compartment is considered an anaerobic one (without airflow supply) for the whole duration of the cycle since the presence of air is limited there even during high aerating conditions under which air volume fractions of up to only 0.004 are observed. Nevertheless, high DO concentrations can be still possible in this compartment (especially close to the surface) during the aerobic phase due to the mixing effect. This was confirmed in an experiment by the DO measurements close to the surface and center of the bioreactor which showed up to 0.5 mg/L lower concentrations than the rest of the tank. Moreover, it was observed that the flow rates in the circular direction are significantly higher than the ones in the radial direction even during the aeration phase (31.2–45.5 m^3/s compared to 0.2–.6.1 m^3/s, respectively). While during the anaerobic phase velocities of between 0 and 0.1 m/s are observed in the stagnation zone, they are increased to almost 0.35 m/s in most cases during the aeration phase which is still significantly lower than the 0.8 m/s in the rest of the tank. The tank is thus divided into three compartments in total; a compartment representing the stagnation zone in the centre during the anaerobic phase, a compartment representing the part of the bioreactor without diffusers where the inflow is located, and a compartment representing the rest of the bioreactor.

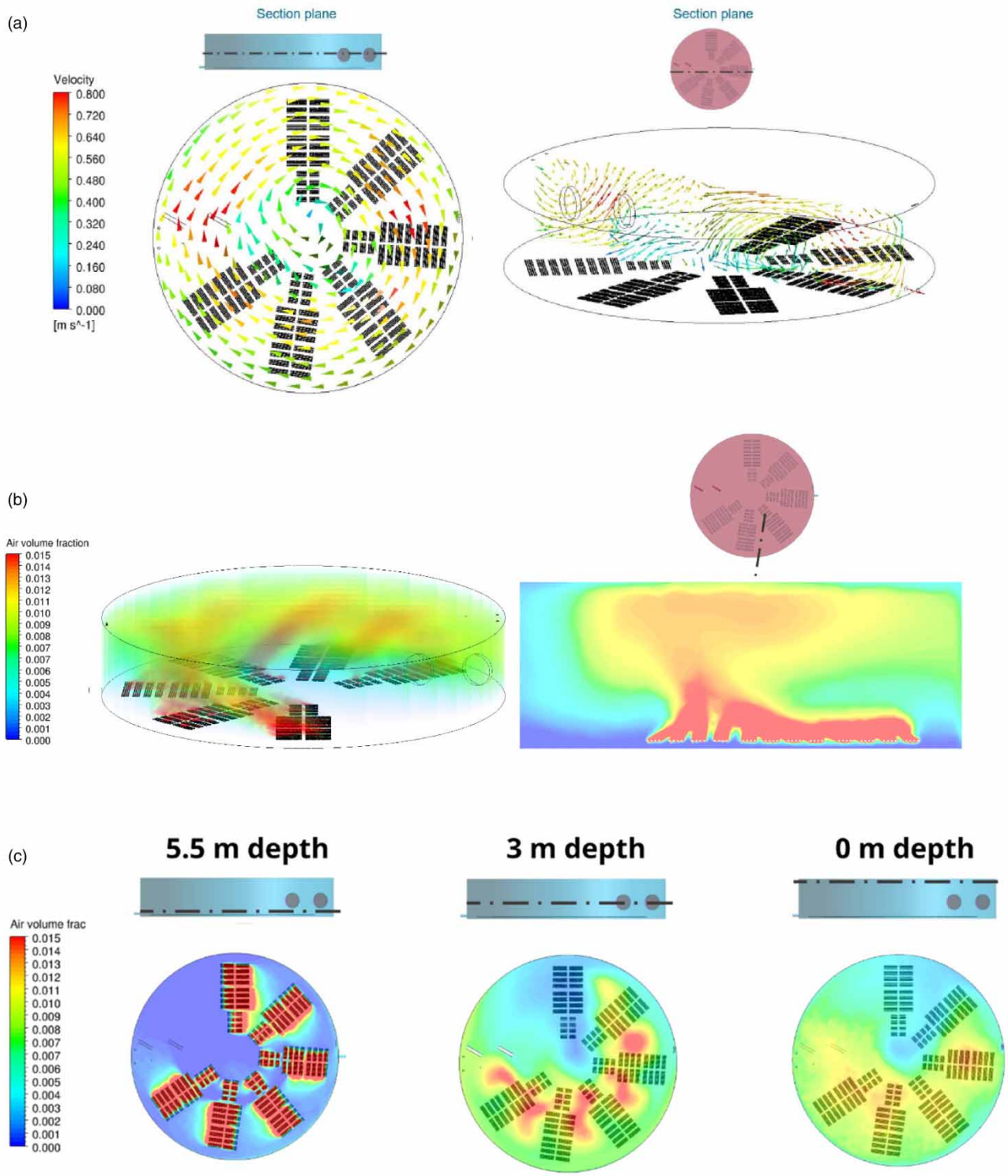

Figure 5 | (a) The velocity vectors simulated with the CFD model for the aerobic phase of the SBR. (b) The air volume fraction simulated with the multi-phase CFD model during the aerobic phase. (c) Comparison of the air volume fraction simulated with the multi-phase CFD model at different depths within the bioreactor.

To capture changes in mixing behaviour between the aerobic and anaerobic phases, the exchange flows between the compartments are modified dynamically according to the SBR cycle. This takes into account the fact that the stagnation zone in the middle of the bioreactor remains somehow separated from the rest of the tank during the anaerobic phase but presents a

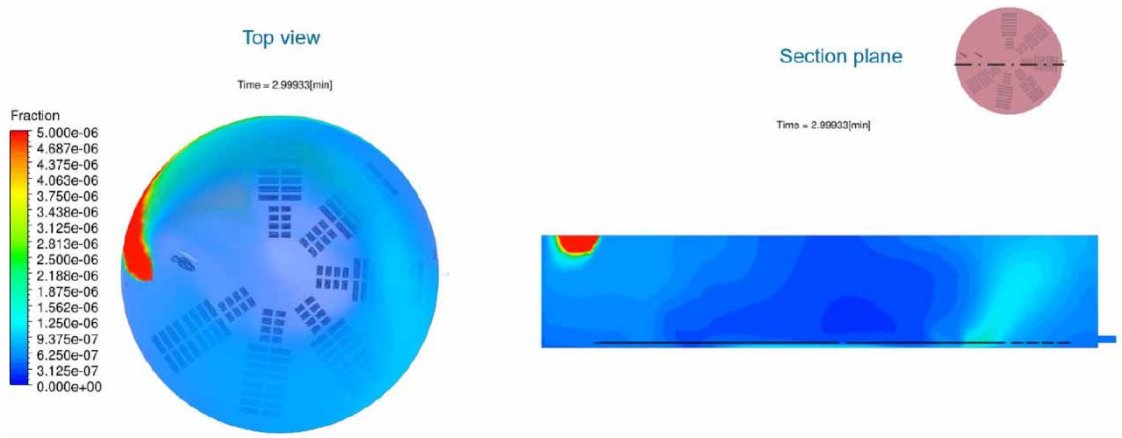

Figure 6 | The result of the transient CFD simulation for the dispersion of FeCl3 injected during the aerobic phase at time = 3 min after the start of the simulation.

much better exchange of flows with other parts during the aerobic phase. Figure 7 shows the scheme of the compartmentalisation during both anaerobic and aerobic stages as well as the volumes and exchange flows of the compartments.

The dynamic CM was implemented in the WEST using CSTRs and exchange flows between them. Additional 'flow controllers' were implemented to change the exchange flows between the compartments based on the time of the SBR cycle. The schematic layout of the model in WEST is depicted in Figure 8. The DO measurements for the controllers are taken from the second compartment (CM_2) where in reality the sensor is located near the inlet of the bioreactor. On the other hand, the aeration is supplied to the first compartment (CM_1) where the diffusers are located in the real SBR reactor.

Figure 9 shows the results of the 2-day dynamic simulation comparing measurement data to the single-CSTR model and the CM model in which the CM configuration is dynamically switched between the anaerobic and aerobic phases of the SBR cycle. Both DO and PO4 measurement data are taken from the probes located near the inlet of the bioreactor which in

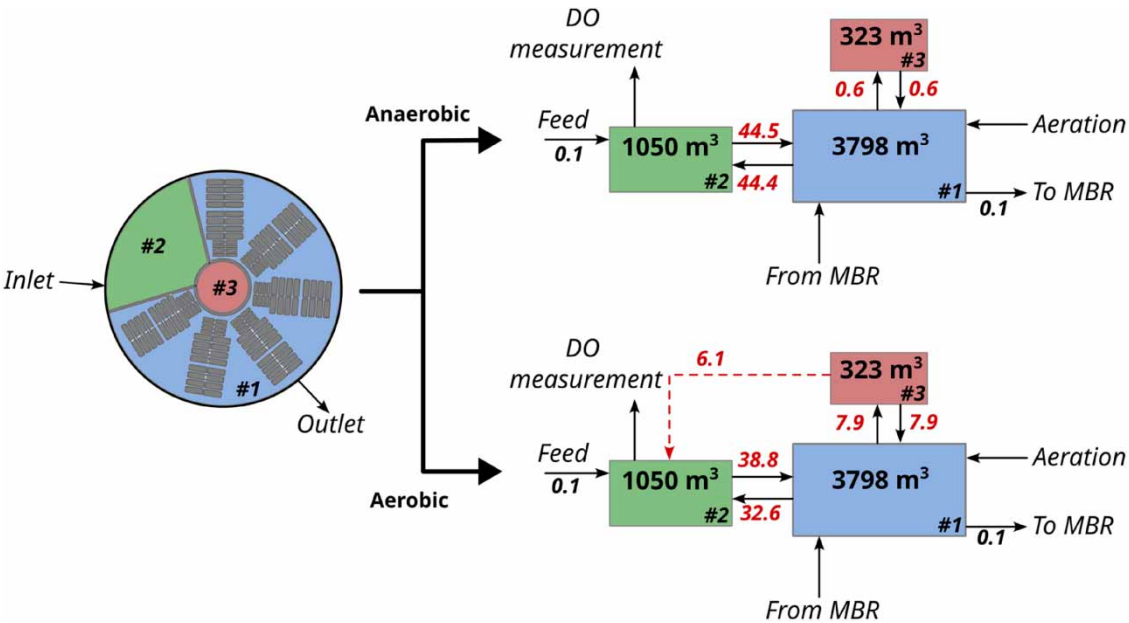

Figure 7 | The scheme of the compartmentalisation of the SBR. The flow from CM_3 to CM_2 (dashed line) is active only during aerobic phase. Measurements are taken from compartment 2 and the air flow is supplied to the compartment 1 while the compartment 3 represents the central stagnation zone during the anaerobic phase. All flow rates reported in the figure are in m^3/s.

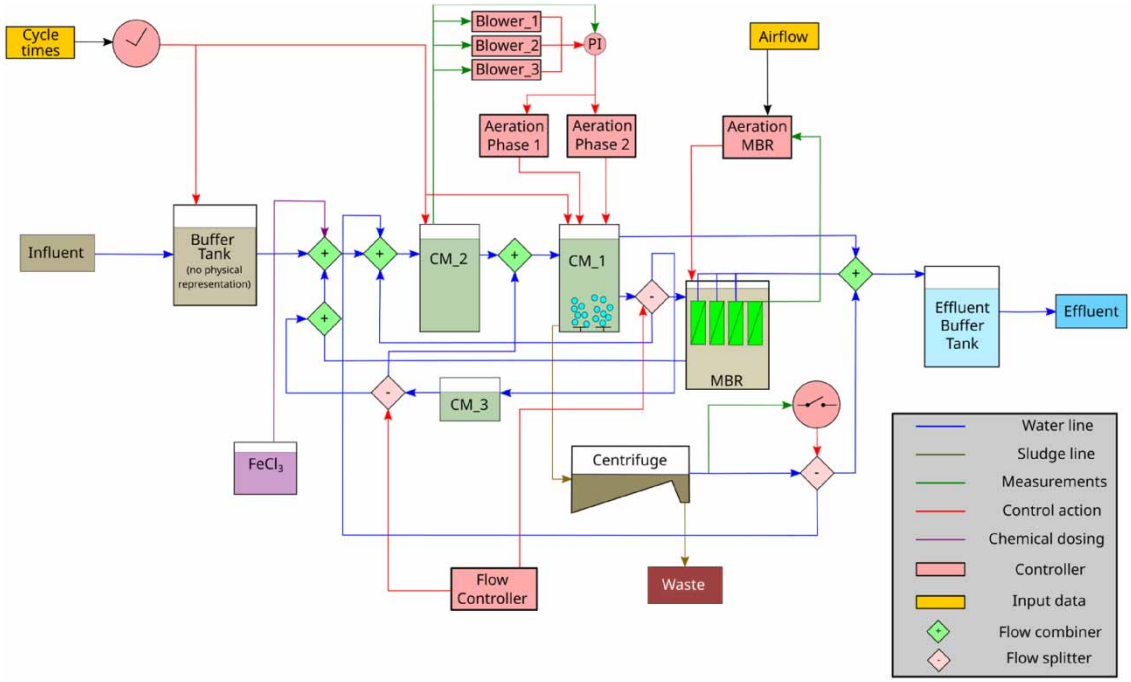

Figure 8 | The schematic layout of the implemented compartmental model in WEST.

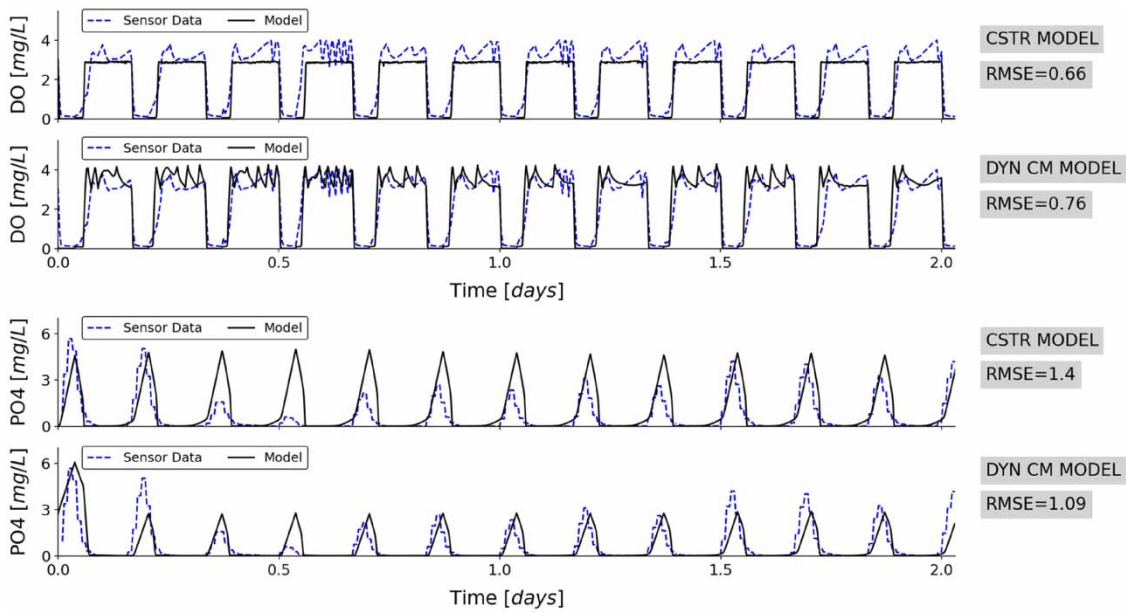

Figure 9 | The results of the dynamic WEST model simulation for DO and PO4 comparing the CSTR model with the CM.

the dynamic CM refers to the CM_2. All the parameters of the biokinetic model are the same in both models which means they are at the calibrated values reported in Table 2. A significant improvement can be seen for the DO and PO4 predictions without further calibration of the biokinetic or the aeration model of the single-CSTR configuration. Although the RMSE values for DO do not show a big difference (and for the dynamic CM it is slightly higher), the dynamic CM is capable of capturing the dynamics of DO during the aeration phases which was something that the CSTR model was not able to do despite of the extensive calibration efforts done on the biokinetic and aeration models and the detailed implementation of the DO

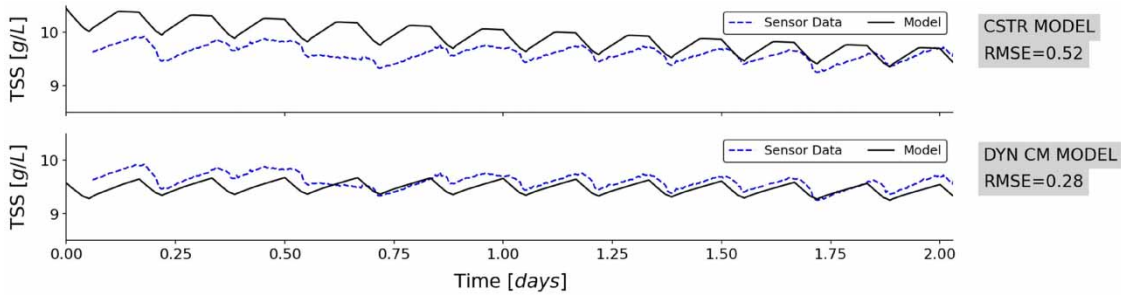

Figure 10 | The results of the dynamic WEST model simulation for TSS comparing the CSTR model with the dynamic CM.

control strategy. In addition, the phosphate predictions which were overestimated in most cycles in the CSTR model, are fitting the measurement data in a better way by reducing the RMSE from 1.4 to 1.09. However, small dynamics between the cycles are still not being captured in detail.

In the single-CSTR model, there is no distinction between where the DO sensor is located, where the the inlet/recycle flows are located, where the sludge is taken out of the tank, and where the airflow is supplied to the bioreactor. Whereas the dynamic CM describes these elements in a more realistic way by separating the point of DO measurement from the injection of air as well as the point of sludge removal and inlet/recycle flows. The sensor location was proven to be an important aspect to consider (Rehman *et al.* 2014). The overestimation of the phosphate in the single-CSTR model shows that the model predicts a higher release of phosphate during the anaerobic phase compared to the data. Considering the stagnation zone in the middle of the bioreactor during the anaerobic phase, it makes sense that the phosphate release would not be the same in all regions of the tank and if in theory higher phosphate can be released in the ideal case (which is represented by the single-CSTR model), in reality the measurements by the probe near the inlet would be lower due to the incomplete mixing and much slower transport of the flow from the middle to the rest of the reactor. This can explain the overestimation of the phosphate in the single-CSTR model.

Looking at the TSS in the SBR (Figure 10), the single-CSTR model shows a relatively good capture of the dynamics but the solids remain constant during the second aeration phase (without feeding). This can be explained by the DO profile that does not show any dynamics during the aeration phase and consequently leads to no further biomass growth in the bioreactor. On the other hand, the improved prediction of the available DO in the SBR for the dynamic CM model also noticeably changed the profile of the TSS bringing the simulation results much closer to the actual measured dynamics.

Overall, the dynamic CM model was able to improve the predictive power of the mechanistic biokinetic model compared to the single-CSTR model without further recalibration needs. The dynamic CM developed in this study not only provides an addition to the scarce literature on CM in the wastewater domain but also presents its application for a non-continuous process (within the operation of the SBR) which is prone to high variations in the mixing patterns during different cycle phases. Moreover, it investigates the impact of hydrodynamics on biological phosphorus removal where no previous studies using CM have been documented. This proves once again the importance of hydrodynamics and shows how CM can be a valuable approach to improve the model's predictive power in mechanistic biokinetic models. Considering the emergence of DTs and their need for long-standing reliability and the potential requirement for frequent validation/recalibration of (Torfs *et al.* 2022), a CM can provide a more accurate representation of the hydrodynamics (compared to the conventional CSTR or TIS approaches) and therefore reduce the constant effort to compensate for the errors caused by the structure of the model.

CONCLUSIONS

Systemic approaches based on ideal reactors (such as in TIS configuration) for the wastewater treatment bioreactors are too simplistic and inaccurate for describing such systems when they are significantly affected by non-ideal mixing patterns. Even though CFD models can provide a highly accurate representation of the hydrodynamics for the bioreactors, they are computationally too expensive to be used for the emerging DT applications which require real-time simulations. Compartmental models can be considered as the middle-ground solution. They provide a more accurate representation of the reactor mixing conditions while still being computationally affordable. Nevertheless, their applications in the wastewater domain

are limited and the available literature on the subject is more focused on the continuous flow reactors and the impact of incomplete mixing on the COD/N biokinetics.

This study presents the development and implementation of a dynamic CM for a SBR treating maltery wastewater focusing on the biological phosphorus removal process. The CFD simulations of the various stages of the SBR cycle helped in building a CM with three distinct compartments that dynamically vary the exchange flows between the compartments to adapt to the mixing conditions occurring during the anaerobic and aerobic phases of the cycle.

The results of the dynamic CM simulations show significant improvements in the predictive power of the model for DO, PO_4 and TSS concentrations in the SBR over the overly simplified single-CSTR model without further recalibration of the underlying mechanistic biokinetic model.

DATA AVAILABILITY STATEMENT

Data cannot be made publicly available; readers should contact the corresponding author for details.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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