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Next-generation compartmental models for applications in Digital Twinning of WRRFs

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Introduction

The Tanks-In-Series (TIS) approach is widely used by the wastewater treatment modelling community to model the hydrodynamics of (large) bioreactors. This approach assumes that local recirculation and concentration gradients are negligible by averaging out variations in dimensions perpendicular to the bulk flow direction. This assumption can be questioned for modelling full-scale WRRF bioreactors where “ideal” plug flow behaviour is rare to occur. To tackle this, Computational fluid dynamics (CFD) can be used to describe the hydrodynamics of the bioreactor with a high level of detail (Rehman, 2016). However, there are obstacles to the more widespread application of CFD and CFD-biokinetic models, such as high computational costs, especially for applications in dynamic flow sheet models (De Mulder, 2019). Compartmental Model (CM), initially suggested by De Clercq et al. (1999) and Alex et al.(1999), is the middle ground between the simplicity of TIS and the complexity of CFD, in which a reactor is modelled as a conceptual network of CSTRs connected by convective and exchange fluxes. The size and number of compartments can be derived from a detailed CFD model. A CM presents a more realistic representation of the mixing behaviour inside bioreactors compared to the conventional TIS. This helps avoid unnecessary and erroneous calibration efforts of other model parameters, thus improving the predictive power of the models. Moving to the digitalization era and introducing Digital Twins (DT) in WRRFs, CMs could provide a significant advantage over conventional models by reducing the need for frequent validation/(re)calibration of the models, leading to higher trust by plant operators. In addition, CMs are significantly less computationally expensive than CFD models, which are still not adapted for the real-time operation of DTs.

As one of the first attempts to implement CM in full-scale WRRFs, Rehman (2016) developed a CM based on a CFD-biokinetic model for the aeration tank of the Eindhoven WRRF in The Netherlands. This CM was implemented by De Mulder (2019) in a plant-wide model showing superior model prediction power for some key variables at almost equal simulation time as the TIS model. However, despite these model improvements, the plant still struggles with less good predictions of denitrification performance under wet-weather conditions, which hamper the plant’s plans to move toward a Digital Twin. A possible reason for this could be the location of the return sludge pipe in the anoxic reactor. As the return sludge is fed to the bottom of the reactor, this might cause sludge stratification between the bottom and the top of the reactor (since the density of the RAS is significantly higher than the AS, given its higher concentration), thus deviating significantly from the completely mixed assumption as rection rates will be heteregeneous. Therefore, in this study, a CFD model was developed to investigate the mixing behaviour in the anoxic tank, and a CM model was developed to improve the predictions of denitrification behaviour of the full-plant model.

Description of the WRRF and plant-wide models

The Eindhoven WRRF is the third-largest WRRF in the Netherlands, with a treatment capacity of 750,000 P.E. operated and managed by Waterboard De Dommel. It biologically removes carbon, nitrogen and phosphorus in three parallel lines with a modified University of Cape Town (UCT) configuration with a maximum hydraulic capacity of 26250 m^3/h. Each circular biological tank has inner, middle and outer rings corresponding to anaerobic, anoxic and partially aerated units, respectively. The return activated sludge (RAS) goes from the secondary settling tank to the anoxic middle ring. Nitrate is being recycled from the outer ring to the anoxic middle ring, and there is also a recycle from the anoxic to anaerobic ring. The plant-wide model of the Eindhoven WRRF (implemented in WEST, DHI) has been calibrated and validated based on almost a decade of extensive modelling efforts. The model was initially developed with a TIS approach (4 anaerobic, 2 anoxic and 6 aerobic tanks), modelling one line of treatment with a total volume equal to all three lines combined (TIS-model). It was further extended to a CM of the aeration tank (CM-AR) (De Mulder 2019). The data used for the calibration and validation of models were collected from 16th November to 8th December 2013 (day 320 to 342). This 22-day long dynamic dataset represents both dry and wet weather conditions.

CM-ANX development

The extension of the CM to the anoxic tank was developed based on a CFD-biokinetic simulation (performed in ANSYS FLUENT). An apparent sludge stratification effect in the bioreactor could be observed in CFD results and measurement campaigns. Two compartmentalization schemes were developed considering the velocity vector and TSS concentration obtained from the CFD model as governing parameters. It was found that the CM based on velocity vectors could capture an improved dynamic of solids in the reactor since they incorporate the effect of viscosity variations created by incoming RAS flow as concentrated and relatively denser biomass streams into the reactor. Based on the procedure reported in Rehman (2016) using the Cumulative Species Distributions (aka Rehman-Nopens curves), five longitudinal compartments were considered, each divided into three radial compartments. Additionally, one of the compartments was divided along the height to account for the RAS entry point resulting in a total number of 16 compartments representing the anoxic middle ring (Fig.1). The CM was then incorporated into the plant-wide model in which the aerobic outer ring was previously modelled with the CM approach.

Results and Discussion

Figure 2 demonstrates the validation plots comparing the simulation results of TIS, CM-AR and CM-ANX models. For the MLSS concentration in the biological tanks, TIS and CM-AR models gave comparable results predicting the range of solids accurately enough during dry weather condition.

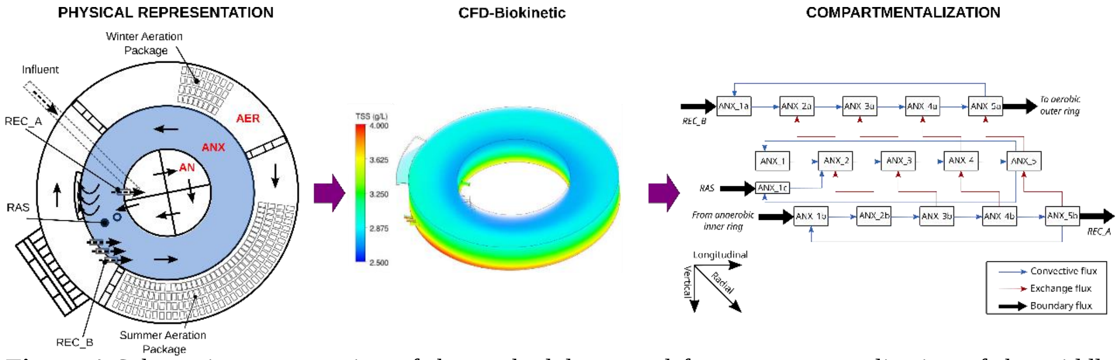

Figure 1 Schematic representation of the methodology used for compartmentalization of the middle (Anoxic) ring of the Eindhoven WRRF

However, neither model could capture the dynamics and effect of a wet weather event on solids. Previously several attempts have been made to resolve these issues by trying different settling models, which were unsuccessful. Eventually, an empirical settler model was developed to improve the model's predictability during wet weather conditions (De Mulder, 2019). The CM-ANX model shows some improvement in capturing the dynamics during dry weather (although slight overestimation can be seen in the period of 325 to 330), but it shows far superior performance in capturing the peaks during wet weather conditions. This is also reflected in the average mean relative errors (AMRE), which shows a slight increase for the overall period but improvements when considering only the wet weather period. The solids stratification and concentration gradient due to the incoming concentrated RAS flow increases the viscosity, impacting the velocity gradients. These hydrodynamic features are captured by the CFD-biokinetic model (see Fig. 1) and translated into the CM-ANX model. An important aspect here is that building the CM directly based on the TSS profile from the CFD-biokinetic output was unsuccessful. The CM was built on the velocity vectors since they incorporate the effect of viscosity variations on the mixing pattern. Hence, while the reactor volume remains unchanged in the construction of the CM, the structure of the CM leads to a more realistic retention time and TSS dynamics. It should be noted that the uncalibrated Bürger-Diehl settler model (Bürger et al., 2013) was used with the default parameters in all three models. This highlights that detailed hydrodynamic information could avoid unnecessary numerical tuning/calibration and impose further complexity on the model structure using the empirical settling model.

Regarding the nitrate concentrations in the anoxic reactor, it can be seen that both CM-AR and CM-ANX models yield better predictions than the TIS model. The AMRE significantly improved from TIS (53%) to CM models (33-34%). Also, going from CM-AR to CM-ANX only shows a slight improvement in the AMRE values. However, the impact of the new CM model on the dynamic pattern of nitrate is more pronounced. The regions where nitrate concentrations are underestimated in the TIS and CM-AR model (see the period between day 325 and 328) can be linked to an underestimation of the nitrate production due to the TIS and CM-AR models' inability to capture the actual residence time in the anoxic zone. Hence, it can be concluded that by increasing the hydrodynamic detail in the model structure, predictions for TSS and nitrate dynamics improved significantly, reaching a higher predictive power for the model to be used in digital twin applications. The CM-ANX predictions show high-frequency dynamics in some periods, which can be linked to the chosen model solver and the increased stiffness of the model structure compared to the other two models.

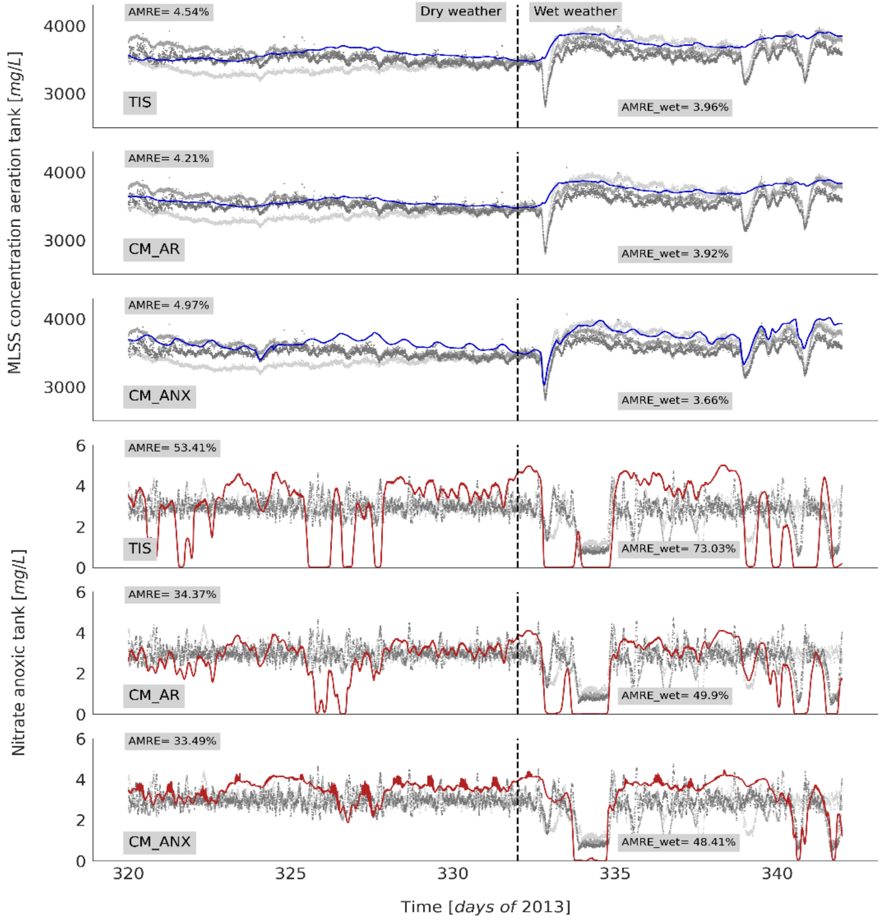

Figure 2 Model predictions for MLSS (blue on the top) and nitrate in the anoxic reactor (red on the bottom) for the TIS, CM-AR and CM-ANX models (solid lines) and online measured data for the three treatment lines (grey dots). AMRE: average mean relative error (over three lines).

Conclusion and Opinion

One of the bottlenecks of mechanistic plant-wide water resource recovery facility (WRRF) models commonly used in most of the available digital twin (DT) cases relates to the level of hydrodynamics details included in these models. They often neglect detailed hydrodynamics of the reactors and simplify the mixing behaviour by the Tanks-In-Series (TIS) approach. In this study, a compartmental model (CM) based on an integrated hydrodynamic-biokinetic model was developed to describe the hydrodynamics of an anoxic reactor of a full-scale water resource recovery facility (WRRF). The results presented in this study highlight the importance of local density variations as a function of suspended solids to improve the model's predictive power and avoid unnecessary calibration of the model parameters. There are likely many plants that have a RAS returning from the bottom of a bioreactor, leading to stratification and hence, non-ideal reactor performance. This will hamper DT development for these plants but can be solved by introducing a CM.

The availability of a model with sufficient predictive power responding to new scenarios and disturbances without frequent validation/(re)calibration is a necessity for the transition to DT applications and the use of models as a real-time decision support tool for the WRRFs. In addition, the computational demand of CFD models is a bottleneck for their application in the real-time operation of DTs and extensive scenario analysis. It is believed that compartmental modelling based on the methodology presented in this study can open a whole new array of advantages, from more prediction power than conventional TIS models to less computational demand than pure CFD models, which can form the new basis for WRRF models implemented in the context of DT.

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