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Elucidating the effects of mixing on nitrous oxide emissions using computational fluid dynamics in a full scale WWTP

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Summary of key findings

Nitrous oxide production within wastewater treatment processes depends largely on the local dissolved oxygen concentrations, which are highly dependent on the extent of mixing in large bioreactors. Current models lack the level of detail needed to account for mixing effects on dissolved oxygen levels. In order to properly address mixing issues, Computational Fluid Dynamic (CFD) modeling was integrated with a biokinetic nitrous oxide model for a full scale municipal wastewater treatment plant. The model includes nitrous oxide production from both ammonia oxidizing bacteria denitrification, and heterotrophic denitrification. Results of the combined CFD – biokinetic model are presented and are compared to the performance of traditional simplified models and evaluated based on expert judgment and currently available data. The model results prove that regions of bad mixing clearly influence the overall process rates and predicted N_2O production.

Background and relevance

Greenhouse gas emissions from wastewater treatment plants (WWTP) are a matter of growing concern. The global warming potential of nitrous oxide (N_2O) is 298 times greater than carbon dioxide (IPCC, 2013). Therefore, research on N_2O emissions has become a point of attention in recent research. N_2O production within the wastewater treatment process can be related to different biochemical pathways such as heterotrophic denitrification (von Schulthess et al., 1994), AOB (ammonia oxidizing bacteria) denitrification (Bock et al., 1995) and from PAOs (phosphorous accumulating organisms) (Ahn et al. (2001). Several modeling studies have been performed to quantify N_2O emissions taking different pathways into account (Hiatt and Grady 2008, Flores-Alsina et al. 2011, Ni et al. 2013, Mampaey et al. 2013 and Guo & Vanrolleghem 2013). Common consensus is found on Hiatt and Grady's ASMN model of four step heterotrophic denitrification which includes N_2O as an intermediate. Mampaey et al. (2013), on the other hand, also included N_2O and nitric oxide (NO) production due to AOB. From these studies it is understood that dissolved oxygen (DO) plays a key role in quantifying N_2O production and, hence, emissions. Oxygen in wastewater treatment systems is provided by aeration, which is both a source of oxygen and mixing. Current modeling techniques using systemic models do not take local mixing into account and thus average out local variations in predicting concentrations. These systemic models are calibrated by changing the kinetic parameters such as half saturation coefficient of oxygen and ammonia (Arnaldos et al. 2014). Recent studies have shown that there might be other phenomenon, such as mixing, playing a vital role in predicting the true concentrations (Arnaldos et al. 2014). Computational Fluid Dynamics (CFD) is a method able to account for spatial effects and study the influence of design parameters and phenomena at local scale. Studies have shown more improved systemic model structures can be obtained using CFD (Le Moullec et al. 2010a). Moreover, Rehman et al. (2014) have integrated hydrodynamic and bio-kinetic modelling using activated sludge model No. 1 (ASM1) for a full scale WWTP. This contribution extends the latter by incorporating models predicting nitrous oxide concentrations.

Material and methods

This study is performed on one of the aeration tanks (AT) of the wastewater treatment facility in Eindhoven (The Netherlands). It concerns the outer ring of a circular carrousel type bioreactor, where mixed liquor enters from the middle anoxic ring and leaves the reactor at the bottom after passing through the whole reactor in the clockwise direction (Figure 1(a)).

We extended the model of Rehman et al. (2014) with current nitrous oxide models from the literature, i.e. including heterotrophic denitrification (Hiatt & Grady 2008), AOB denitrification (Mampaey et al. 2013) and DO Haldane kinetics (Guo and Vanrolleghem 2013). The biological components are integrated with the hydrodynamic model using 18 user defined scalars. Steady state CFD simulations were performed using the influent flow and composition, collected from specific WWTP data, as inlet boundary conditions. Default kinetic parameter values were adopted from Guo and Vanrolleghem (2013).

Discussion

The purpose of the simulations was to see how local mixing impacts the local N_2O concentrations. In this context, Figure 1(b) shows the velocity vector plots in the vertical cross section of the reactor (in the aerated region). This clearly shows macromixing patterns with 2 major "dead" zones which exhibit reduced mass transfer. These regions are averaged out when using simpler models (such as tank-in-series modelling). Figure 2 shows the concentration plots for different biological components. The non-uniform behavior is quite evident and impact of dead zones on the local concentrations of oxygen, ammonia and nitrous oxide can be observed. Dissolved oxygen concentration varies from 0.14 to 2.25 mg/L in the aerated region and subsequently nitrous oxide concentrations range between 0.05 – 0.29 mg/L. It is obvious from these preliminary results (obviously needing validation in the future) that integrated CFD models can be very useful and provide detailed information about the system behavior and possible troubleshooting. It would also be interesting to see the impact of varying flow conditions on nitrous oxide production. In the full paper detailed modeling results and system evaluation will be presented as well as comparison with TIS model predictions.

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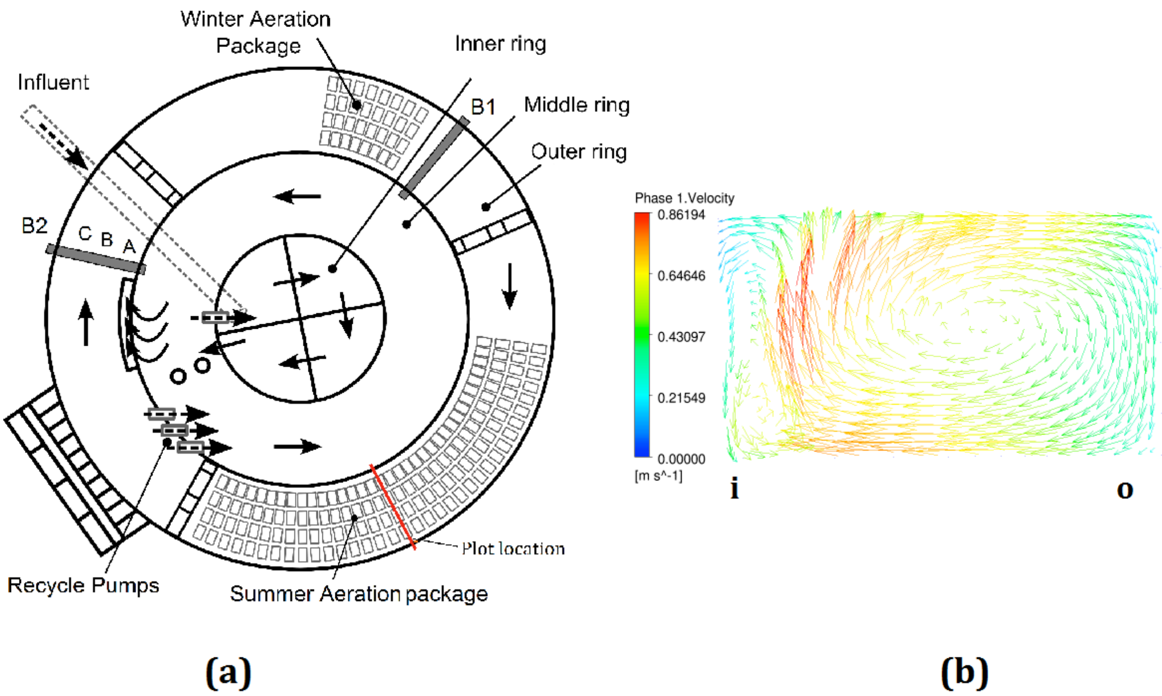

Figure 1 (a) Flow configuration of the bioreactor, (b) Velocity vector plots at the vertical cross section in the aerated region

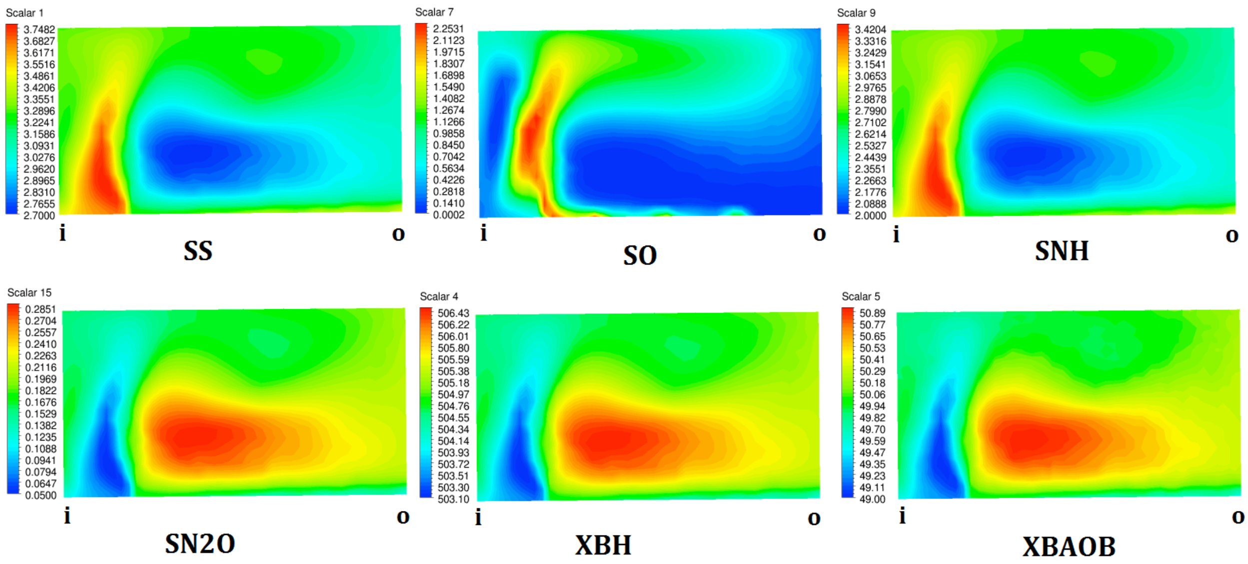

Figure 2 Contour plots for different components (mg/L)

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