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Numerical modelling of N₂O emission from surface aerated oxidation ditch activated sludge reactors

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Abstract: The main aim of this study focuses on the feasibility of developing and calibrating a simple computational fluid dynamics (CFD) model – single-phase, three-dimensional (3-D) – to predict nitrous oxide (N₂O) emission from an activated sludge oxidation ditch. The additional aim is to assess the relative importance of design and operational boundaries to N₂O emission was answered using a validated CFD tool. The NDHA model was implemented to describe the reaction kinetics involving N₂O production. A method is developed for calibrating the mass transfer models for oxygen (alpha factor) and N₂O.

Keywords: Computational fluid dynamics (CFD); Activated sludge wastewater treatment; Nitrous oxide emission; Sensitivity analysis

Introduction

The effective numerical prediction of nitrous oxide (N₂O) emission – a potent greenhouse gas – from biological wastewater treatment plants (WRRFs) represents a significant knowledge gap in literature that can lead to developing more effective mitigation measures – in terms of reactor design and operation – for water resource reclamation facilities. For that improvement in on-line monitoring (especially for N₂O) of full scale WRRF should be developed in the future (Mannina et al., 2016).

The main aims of this study include (i) developing and calibrating a three-dimensional, single- and two-phase CFD simulation models of an activated sludge oxidation ditch by combining online monitoring data with hydrodynamics, gas mass transfer and the NDHA biokinetic models; (ii) developing a practical method to estimate the alpha factor and the k_{LA} for N₂O using experimental and CFD simulation data; (iii) evaluating the CFD tool using long-term full-scale measurement data; and (iv) scenario simulations aiming to statistically screen and discriminate design and operating boundary conditions conducive to enhancing N₂O emission.

Material and Methods

Oxidation ditch design and data collection. The CFD simulation model was developed and calibrated using real data obtained in the Lynetten WRRF, Denmark. The geometry was created in DesignModeller-ANSYS® (Fig. 1). There are two surface aerators installed in the ditch. Simulations presented here focused only on the aeration operation phase. In the Lynetten WRRF, sensors were introduced for recording the concentration of oxygen and nitrous oxide (Fig. 3a-b).

The biokinetic model. The NDHA model is employed to describe the biokinetics of N₂O production (Domingo-Félez and Smets, 2016; Domingo-Félez *et al.*, 2017). The model accounts for N₂O production via nitrifier nitrification (N), nitrifier denitrification (D), heterotrophic denitrification (H) and abiotic reactions (A).

CFD simulation. All gases were assumed to be dissolved in the liquid phase so that the assumption of single-phase flow was made for simplification. The 3-D simulations were carried out using the software CFX-ANSYS® (Release 19.1). The turbulence model used during the simulation was shear stress transport (SST) model.

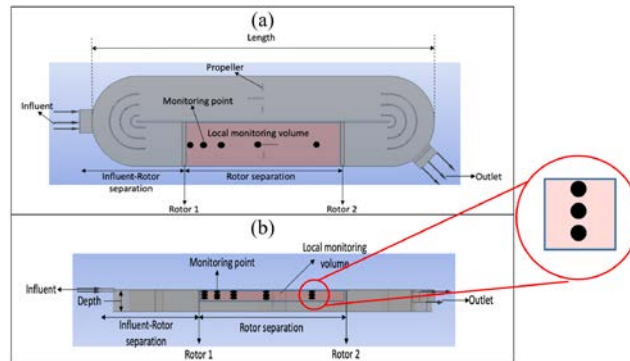


Figure 1 The design layout of the oxidation ditch in Lynetten WRRF - (a) top view and (b) side view. Full-scale sampling points are shown with pink.

Sensitivity index. To assess the relative sensitivity of selected CFD simulation outputs – defined in Fig. 4 – to selected design and operational boundary conditions, local sensitivity indices were calculated using a 2-level fractional factorial design. 16 CFD simulations were carried out using the validated simulation model by considering 9 design and operational boundary conditions. The regression plane (Y) is defined as

$$Y = b_0 + \sum b_i f_i \quad (3)$$

where f_i is the design or operational factor, b_i denotes the respective sensitivity indices, and b_0 represents the intercept. The rankings of normalised sensitivity indices (β_i), calculated as $\beta_i = b_i/b_0$, are plotted for the selected simulation outputs (Guyonvarch *et al.*, 2015).

Method development

For the estimation of the alpha factor (α)

$$\alpha = \frac{K_L a_{O_2} \text{ in wastewater}}{K_L a_{O_2} \text{ in clean water}} \quad (1)$$

and the mass transfer coefficient for N_2O (K_{L,N_2O}) a combined experimental and numerical method was developed, which is briefly spread out here. Values of K_{L,N_2O} was measured (Fig. 2a) at five different monitoring points (Fig. 1) downstream to one of the surface aerators using gas sensor data obtained using the flux chamber technique (Ekström *et al.*, 2017). Values of $K_{L,A}$ for oxygen in clean water ($K_{L,A_{O_2, \text{clean}}}$) was obtained by predicting dissolved oxygen concentration evolution at the same monitoring points as K_{L,N_2O} using the CFD tool, simulating a re-aeration test (Fig. 2b). We note that, in a single-phase CFD model, the lack of bubble size distribution can introduce significant error in the estimation of kla_{O_2} – and thus in the Kla_{N_2O} – because gas mass transfer can significantly change over depth. The single-phase simulation model is developed as a benchmark to assess the structural complexity and its impact on predictive accuracy and sensitivity rankings for design and operational parameters. Meanwhile, an empirical function was inferred to describe the correlation between K_{L,N_2O} and $K_{L,A_{O_2, \text{clean}}}$ intensive parameters using measured data obtained in targeted laboratory-scale measurements (Domingo-Félez *et al.*, 2014) as:

$$K_{LA}N_{2O} = [\epsilon \cdot \ln(K_{LA}O_{2, \text{clean}} \cdot \alpha) + \gamma] K_{LA}O_{2, \text{clean}} \cdot \alpha \quad (2)$$

where ϵ and γ denote correlation parameters. Values of the α factor were calculated by fitting Eq. 2 to the measured $K_{LA}N_{2O}$ data, and, as a simplification, the α factor is assumed to be constant.

Results and Discussion

Values of $K_{LA}O_{2, \text{clean}}$ were estimated in five spatial points (Fig. 2a) downstream to one of the surface aerators (Fig. 1). In addition to the five monitoring points, located close to liquid surface (Fig. 2b), $K_{LA}O_{2, \text{clean}}$ was estimated at two additional vertical points defined for each horizontal location in the CFD domain at 0.5- and 1.0-metre depths. (Fig. 1). The $K_{LA}N_{2O}$ field in the numerical domain is defined as a function of the liquid velocity using a regression model developed, for which simulated flow velocity readings were made at the five monitoring points (Fig. 2d).

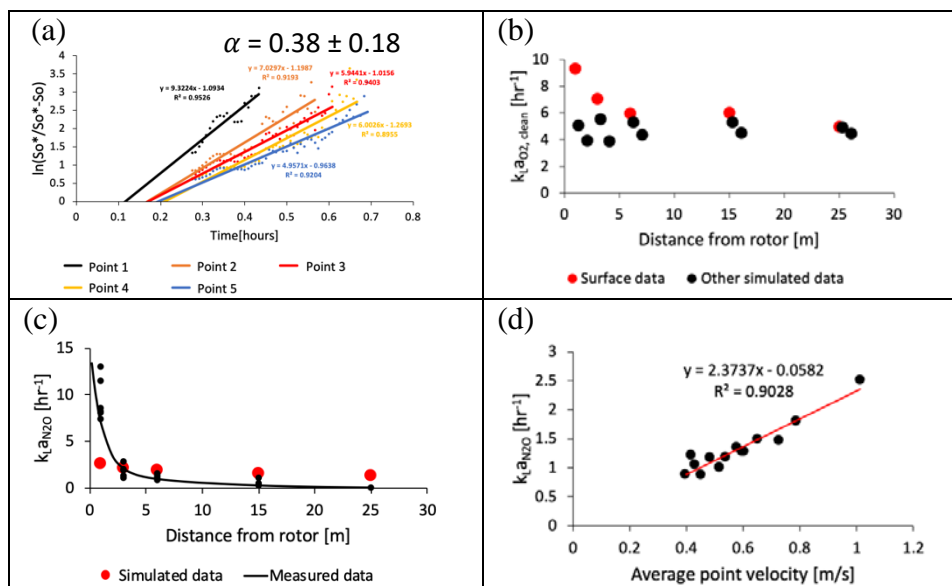


Figure 2 Calibration of the gas mass transfer sub-model – (A) Normalised dissolved oxygen concentration plotted against time obtained in the clean water test CFD simulations; (B) Spatial distribution of $K_{LA}O_{2, \text{clean}}$ values obtained downstream to the rotors; (C) Spatial distribution of measured and simulated $K_{LA}N_{2O}$ values; (D) Regression analysis for $K_{LA}N_{2O}$ as a function of average flow velocity – regression function used in defined regions – downstream to the rotors – of the CFD simulation model to compute N_2O stripping mass transfer.

Average dissolved oxygen and N₂O concentration sensor data (Fig. 3a-b) obtained in the Lynetten oxidation ditch during aeration phases reasonably agree (somewhat lower) with simulation results obtained using the calibrated tool (3-c-d), thus validating the simulation model.

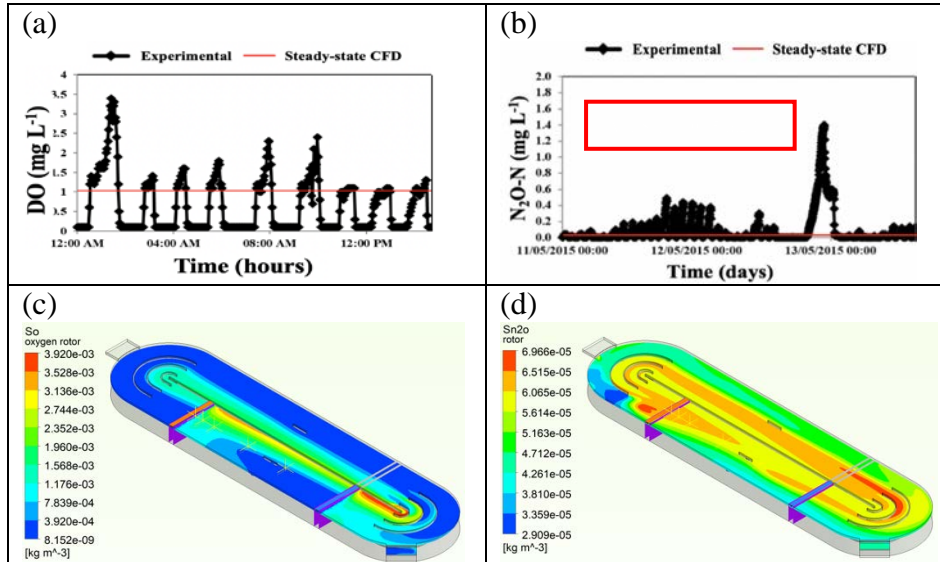


Figure 3 The measured oxygen (A) and N₂O concentration (b) in the Lynetten WRRF, Denmark. CFD simulation results obtained for dissolved oxygen (C) and N₂O concentration (D) fields.

Sensitivity rankings (Fig. 4) obtained using the CFD simulation outputs include N₂O concentration in the surface layer and in the effluent stream, the concentrations of hydroxylamine (NH₂OH) and nitric oxide (NO) in the effluent and the volume-averaged N₂O production rate obtained in the entire reactor volume. Additionally, the volume-averaged N₂O production rates are considered in the screening study. The six most significant parameters found include the reactor L/D ratio, rotor speed, rotor separation distance, influent-rotor separation distance, concentration of input biomass and influent mass flow rate separately. For future study, X_{tin} and Q_{in} will be combined and treated as one parameter, which can be defined as amount of biomass input in the influent.

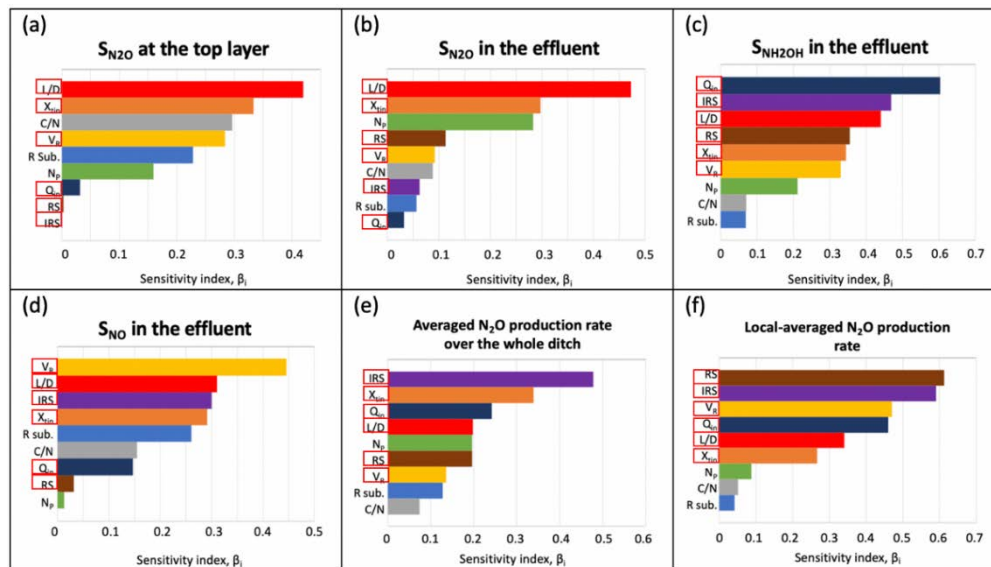


Figure 4 The factorial experimental design (local sensitivity) results related to concentration of N_2O (a) at the top of the oxidation ditch and (b) in the effluent, (c) concentration of NH_2OH and (d) NO in the effluent, (e) the volume-averaged production rate of N_2O in the whole ditch, and the (f) local-averaged production rate of N_2O . The local volume is illustrated in Fig. 1. C/N is COD/N ratio, Q_{in} is volumetric influent flowrate, X_{in} is biomass concentration in the influent, V_R is rotor speed, $R_{sub.}$ is the rotor submergence, N_P is the number of operating propellers, L/D is the length and depth ratio of the oxidation ditch, RS is the rotor separation distance and IRS is the influent and first rotor separation distance.

Conclusions

CFD simulation model developed for predicting N_2O emission from activated sludge oxidation ditch. The simulation model was successfully calibrated using a novel method developed to estimate gas mass transfer model parameters. The factorial screening study indicate significant design and operational parameters – a significant outcome of this study that can lead to improved design and operation of WRRF in the future. Further details, including the development of the two-phase CFD model, amongst others, will additionally be presented at Watermatex2019.

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