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P124 – CFD modelling of N_2O emission from surface aerated activated sludge reactors – Systematic mesh refinement and sensitivity analysis

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Introduction

The effective numerical prediction of nitrous oxide (N_2O) emission – a potent greenhouse gas – from biological wastewater treatment plants (WWTPs) is crucial for developing effective climate change mitigation measures for urban water systems. Based on previous research (Qiu *et al.*, 2019), the novel method for estimating the alpha factor and the stripping gas mass transfer coefficient for N_2O (k_La_{N2O}) was developed using experimental and CFD simulation data. By combining hydrodynamics, gas mass transfer and the NDHA biokinetic model, a three-dimensional, single-phase, CFD simulation model of a surface-aerated activated sludge oxidation ditch has been developed.

The main aims of this study include (i) mesh refinement of the current three-dimensional, single-phase, CFD model by employing the grid convergence index (GCI); (ii) assessing the impact of mesh refinement on predicting N_2O emission from activated sludge reactor; and (iii) quantifying the relative sensitivity of model outputs associated with the prediction of N_2O emission to selected design and flow boundary conditions, thereby identifying areas for improving reactor design and operation.

Methodological Approach

Oxidation ditch design and data collection. The CFD simulation model was developed and calibrated using real data obtained in the Lynetten wastewater treatment plant. The geometry was created in DesignModeller-ANSYS® (Figure 1).

The biokinetic model. The NDHA model is employed to describe the biokinetics of N_2O production (Domingo-Félez *et al.*, 2017). The model accounts for N_2O 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® (R2).

GCI and mesh quality. The Grid Convergence Index (GCI) is a simple method to report grid convergence quality. Normally, the test will be applied to three meshes, which are coarse, medium and fine meshes. The flow velocity at 6 different spatial points (v_i, v_{in}, and v_{out}) are used as simulation monitoring outputs illustrated in Figure 2. $\varepsilon_{i(i-1)}$ is the absolute error between two meshes based on the 6 monitoring outputs. The GCI is calculated based on the comparison of flow velocities between each two meshes. The full mathematic calculation will be provided in the full paper (Roache, 1998; Tanaka, 2014). Based on expert knowledge, the standard GCI for mesh acceptation is lower than 3 (Climent *et al.*, 2019). The Courant number and Yplus are used to assess the mesh quality. Courant number provides a measure of how many nodes is transported per time step, hence, lower Courant number is better with the ideal value being 1. Yplus represents the quality of inflation layer. Low Yplus is desirable as well. The unrefined mesh, which will be mentioned in the results and discussion section, is referred to the unstructured mesh without GCI test.

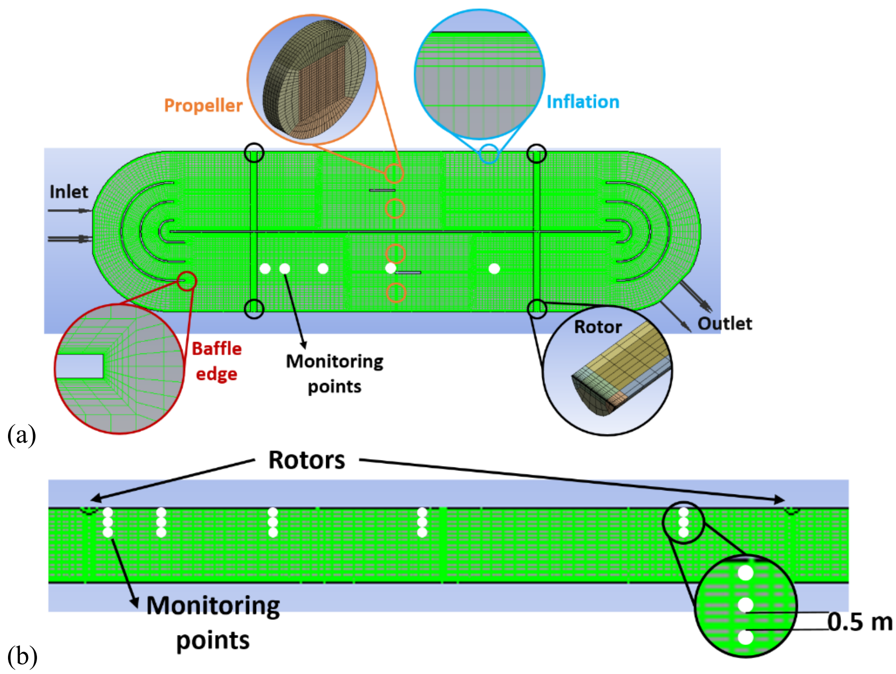

Figure 1 The design layout and mesh of the oxidation ditch in Lynetten WWTP - (a) top view and (b) side section view.

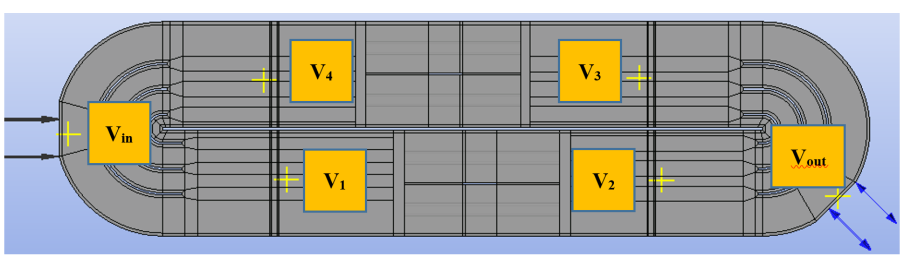

Figure 2 The layout of 6 monitoring points for GCI test.

Results and Discussion

As shown in Figure 1, it can be observed that the geometry had been cut into different sections to refine the mesh into structured elements. Structured mesh can bring high mesh quality and better control of the geometry and inflation layer.

Table 1 illustrates the GCI analysis for three different meshes. The average GCI is around 0.37, which is indicating the mesh to be highly acceptable. The mesh (i = 2) would be chosen because it required less computational time than the fine one, but still can obtain high quality. Table 2 illustrated parameters of mesh quality obtained with unrefined and refined meshes. High orthogonal quality and low skewness are desirable. The orthogonal quality had been increased and the skewness had been decreased after refinement.

Table 1 Overview of the GCI analysis.

i	Elements	v_1 m/s	$\varepsilon_{i(i-1)}$ %	v_2 m/s	$\varepsilon_{i(i-1)}$ %	v_3 m/s	$\varepsilon_{i(i-1)}$ %	v_4 m/s	$\varepsilon_{i(i-1)}$ %	v_{in} m/s	$\varepsilon_{i(i-1)}$ %	v_{out} m/s	$\varepsilon_{i(i-1)}$ %
1	1400000	0.64		0.76		0.64		0.75		0.46		0.56	
2	2500000	0.81	0.21	0.88	0.14	0.80	0.20	0.88	0.14	0.49	0.08	0.57	0.03
3	4200000	0.82	0.002	0.88	0.002	0.82	0.01	0.88	0.003	0.50	0.02	0.58	0.01
GCI		0.01		0.01		0.36		0.03		1.39		0.42	
Average GCI = 0.368													

Table 2 The parameters of the mesh quality before and after the refinement.

	Nodes	Elements	Orthogonal quality	Skewness	Courant number	Yplus
Unrefined	1,398,887	826,260	0.69777	0.30071	> 10	> 1000
Refined (i=2)	3,066,493	2,513,493	0.91718	0.14142	< 5	40 - 80

In Table 2, the courant number and Yplus are all decreased as a result of mesh refinement. The range of Yplus for refined mesh is suitable with $k-\varepsilon$ turbulence model, so $k-\varepsilon$ turbulence model will be used for the refined mesh instead of shear stress transport model, which was used for unrefined mesh (Fig 3c-d) (Qiu *et al.*, 2019).

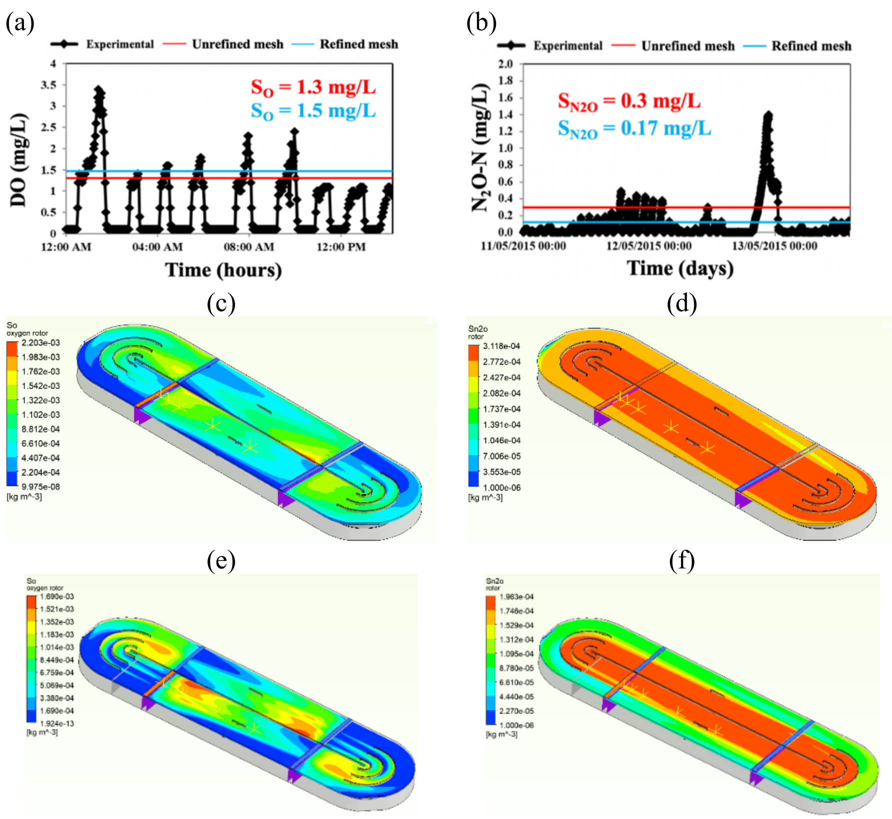

Figure 3 The measured oxygen (a) and N_2O concentration (b) at Lynetten WWTP, Denmark. CFD simulation results obtained with unrefined mesh for dissolved oxygen (c) and N_2O concentration (d) field and with refined mesh (e-f).

Figure 3 shows the results obtained with and the comparison between those obtained using the unrefined and refined meshes. Results from both of meshes (3c-f) were all closely agree with the average dissolved oxygen and N_2O concentration sensor data (Figure 3a-b) obtained in the

Lynetten oxidation ditch during aeration phase. After refinement, DO concentration had slightly increased and N_2O concentration had decreased in half roughly. Furthermore, N_2O concentration data shown in Figure 3f indicate a two-fold difference between the inner and outer regions of the reactor. From this result, it is worth to consider the inner part in optimising the reactor design by controlling the headspace using coverage. Moreover, higher DO and N_2O in the inner region may also suggest that nitrifier nitrification pathway is driving the N_2O emission.

Conclusion

A mesh refinement study was carried out. Additionally, the simulation model developed was successfully calibrated with the refined mesh using measured data. In order to achieve improved reactor design and control in terms of N_2O emission, it is necessary to obtain the significant design and operational parameters. Therefore, sensitivity analysis will be applied to the new refined mesh.

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