Risk assessment modelling of N_2O production in activated sludge systems: Quality not Quantity

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Abstract
A knowledge-based risk assessment modelling approach is proposed to provide a qualitative means of benchmarking WWTP design and control strategies in terms of risk of N_2O production. The approach makes use of ASM model output variables corresponding to conditions that have been specifically linked to the risk of WWTP N_2O production in the literature, and applies a fuzzy logic rule-based system to qualitatively assign risk of N_2O production, as opposed to predicitng actual emission. To demonstrate the proof of concept, the qualitative N_2O risk model was used to interpret mathematical simulation data and distinguish risk of N_2O production resulting from two different aeration control strategies (DO set points of 2 $mg \cdot L^{-1}$ and 1.3 $mg \cdot L^{-1}$). The approach demonstrated its potential in assessing risk of N_2O production on a plant-wide level, as well as the reactor level, which allowed diagnosing specific risks and identifying opportunities for mitigation. Results also demonstrated how the N_2O risk model tool can be helpful in selecting appropriate mechanistic N_2O production models through its risk diagnosis. The N_2O risk assessment model can also serve as a practical decision support tool for qualitatively assessing multi-criteria control strategies as seen in the N_2O risk, effluent quality, and operational cost benchmarking results. The tool is flexible and can be used not only with mathematical model output data, but also online, or SCADA data for examining risk of N_2O production for current and historical plant operations.

Keywords
Activated Sludge Model (ASM), nitrous oxide, qualitative modelling, risk assesment modelling

INTRODUCTION

A considerable amount of focus has been placed on modelling full-scale wastewater treatment plant (WWTP) nitrous oxide (N_2O) emissions in recent years given their high global warming potential. As a result, several promising mechanistic models have been developed (Yu et al., 2010; Ni et al., 2011; Houweling et al., 2011; Law et al., 2012; Ni et al., 2012; Guo and Vanrolleghem, 2013; Mampaey et al., 2013; Ni et al., 2013). However, there is not yet a rigorously validated and consensus-based model. This is largely due to the complex and interactive nature of the processes leading to N_2O emissions from activated sludge systems, including ammonia-oxidizing bacteria (AOB) cell metabolism and gene expressions (Yu et al., 2010, Chandran et al., 2011), AOB and nitrite-oxidizing bacteria (NOB) kinetic rates (Foley et al., 2010), mass transfer processes, and the dynamic operational and environmental conditions that impact the propensity of full-scale microbial populations for producing N_2O during both nitrification and denitrification (Kampschreur et al., 2009; Foley et al., 2010, Chandran et al., 2011). As researchers continue to make strides in reaching a consensus on N_2O dominant pathways, model validation, and implementing and calibrating multiple N_2O pathway models, a knowledge-based risk assessment modelling approach is proposed to complement the progression of the mechanistic description of N_2O production, and provide a qualitative means of benchmarking WWTP design and control strategies. A similar knowledge-based risk assessment modelling approach (AS risk model) has been successfully developed and implemented by Comas et al. (2008) for diagnosing the risk of microbiology related solids separation problems, such as filamentous bulking, foaming, and rising sludge, resulting from various activated sludge control strategies. Parallels between modelling activated sludge solids separation problems and N_2O production, such as the lack of validated mechanistic models and interest in more holistic benchmarking of control strategies, thus motivated the extension of this risk assessment modelling concept for heuristically diagnosing WWTP N_2O production.

METHODS

The methodology for developing the N_2O risk model is generally consistent with that of the AS risk model development (Comas et al., 2008). The proposed integrated mathematical / knowledge-based risk assessment modelling approach makes use of ASM state variables corresponding to conditions that have been specifically linked to the risk of WWTP N_2O production in the literature (Kampschreur et al., 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011), but not yet formalized in a modelling platform through which N_2O risk can be assessed with other criteria in various WWTP simulation scenarios. Therefore, a knowledge base of the operational conditions/parameters associated with risk of N_2O production via heterotrophic denitrification and AOB nitrification/denitrification pathways was compiled and then classified in terms of low, medium, and high risk according to values found in the literature correlating to low, medium, and high N_2O production in either full-scale or lab-scale studies. This knowledge was then represented in a fuzzy logic, IF / THEN rule-based system implemented in both Matlab and Excel, through which a qualitative risk score can be dynamically assigned for each variable representing the operational risk condition. The risk score is based on scale from 0 to 1, with 1 representing the highest risk.

To demonstrate the proof of concept of N_2O risk assessment modelling, the risk model was implemented for only three of the several risk parameters defined in the knowledge base: high nitrite (NO_2^-) for nitrification and denitrification reactors, and low dissolved oxygen (DO) and ammonia oxidation rate (AOR) via DO for nitrification reactors (**Table 1**). This portion of the N_2O risk model was applied to the Benchmark Simulation Model No. 2 (BSM2), a five reactor (two anoxic and three aerobic) MLE configuration. Two different control scenarios were compared: Scenario 1 - DO set point of Activated Sludge Unit (ASU) No. 4 (ASU4) is **2 $mg{\cdot}L^{-1}$**, and Scenario 2 – DO setpoint of ASU4 is **1.3 $mg{\cdot}L^{-1}$**, with k_La set proportionally as $1.5k_La$, k_La, and $0.5k_La$ for the aerobic reactors ASU3, ASU4, and ASU5, respectively. The model implemented in Porro et al. (2011), which includes two-step nitrification and four-step denitrification, was used since the NO_2^- state variable could be used for implementing the N_2O risk model for the high NO_2^- condition, whereas the original BSM2 platform implementing ASM1 only includes single-step nitrification and, hence, no NO_2^- variable. Although the model used in Porro et al. (2011) also includes the implementation of mechanistic models for N_2O production, the N_2O variables are ignored since the purpose of the paper is demonstrating a qualitative approach to assessing control strategies for N_2O production risk as opposed to a quantitative approach (i.e. mechanistically predicting N_2O concentrations). The ASM model output data was then input into the Excel version of the risk model to plot dynamic N_2O risk based upon the corresponding BSM2 model output state variables. Similarly to Corominas et al. (2012) and Guo et al. (2012), Operational Cost Index (OCI), which includes energy costs, and Effluent Quality Index (EQI) per Nopens et al. (2010) were also compared for the two scenarios along with overall N_2O risk to demonstrate the N_2O risk assessment model's potential in multi-criteria decision support.

RESULTS AND DISCUSSION

Table 2 summarizes N_2O risk model results in each of the reactors by average overall risk, from taking the maximum risk of the three individual risk parameters results for each time step, and by percent of time under high risk, with high risk being a risk score of greater than or equal to 0.8, as defined by Comas et al. (2008). Also summarized in **Table 2** is the average overall risk score for all of the reactors, as well as the percent of time under high risk accounting for all reactors, or the percent of the total simulation time in which at least one reactor was under high risk. As anticipated, the two different DO control set points resulted in different conditions in each of the reactors, and hence, noticeable differences in average overall risk scores and time under high risk between the two scenarios. Obviously the largest differences are seen in the aerobic reactors, since the only change between the scenarios was the DO set point. These differences in risk results in the aerobic reactors are due to the DO concentration itself, as low DO implicates the potential for N_2O production via AOB denitrification (Kampschreur et al., 2009; Tallec et al., 2008), and higher DO implicates N_2O production via the hydroxylamine oxidation pathway (Law et al., 2012), as well as the NO_2^- concentrations, which implicate AOB denitrification (Kampschreur et al., 2009). Inspecting the N_2O production risk results in each of the reactors, ASU5 reactor stands out for Scenario 2, with an average overall risk score of 0.95 and 96 percent of the time under high risk.

To give a sense of the N_2O risk model tool's capabilities, **Figure 1** is provided to illustrate further inspection of the risk results, comparing plots of both the individual and overall risk in ASU5 for both scenarios. As the DO set point is lower in Scenario 2, and ASU5 has a k_La that is half that of ASU4 where the DO set point is controlled, it can be understood why the DO levels are significantly lower and hence the N_2O production risk, due to low DO, significantly higher. To add to the risk of ASU5, the lower DO concentrations also lead to higher NO_2^- concentrations compared to Scenario 1 due to the difference in oxygen half-saturation constants between AOB and NOB (Hanaki et al.,1990; Mota et al., 2005), and therefore, higher risk due to high NO_2^- concentrations. As the ASU5 DO concentrations in both scenarios are less than the low risk threshold (<1.8 mg·L^{-1}) for AOR risk, N_2O production risk due to AOR (hydroxylamine oxidation pathway) is always zero in both scenarios for ASU5. As the two remaining risk parameters with high risk values account for AOB denitrification, one could surmise that the particular conditions for ASU5 lend to N_2O production via the AOB denitrification pathway. This highlights the capability of the tool in helping to hypothesize pathways, and therefore, also to select mechanistic models of N_2O production. As the specific risks can be diagnosed, the N_2O risk model tool also demonstrates its potential in identifying opportunities for mitigating N_2O production risk. In this case, it is clear that better control of the DO in ASU5, or better distribution of the air between ASU3 and ASU5 could help to minimize the risk in ASU5, and hence the overall risk for Scenario 2 since ASU5 was under high risk 96 percent of the simulation time. The opportunity to better distribute air among reactors was also noted by Guo et al. (2012) for minimizing greenhouse gas mass transfer and emissions into the air as it is related to the k_La. However, in this case, the N_2O risk model assesses only the effect of DO on risk of production and not mass transfer and emissions. It is also clear from these results that looking at only average overall risk alone, may not fully diagnose the potential N_2O production risk as the average overall risk score for each scenario only differed by 0.07. Since different reactors can be under high risk at different times, it is helpful to also consider the amount of time in which at least one reactor is under high risk.

Table 3 summarizes the N_2O risk, EQI, and OCI results for both scenarios. As anticipated the lower DO control resulted in some cost savings based upon the OCI; however, the EQI decreased slightly, and the average overall N_2O risk score increased slightly. However, the time under high risk for all five reactors increased significantly, by 1.5 times to almost 100 percent of the simulation time. Depending upon objectives, this information could be helpful in determining whether the five percent savings in the OCI is worth increasing the time under high N_2O production risk to almost 100 percent of the time. This information could also help in decision making by prompting further investigation into the conditions in ASU5. For example, if better control or distribution of the air among ASU3 and ASU5 is feasible, as suggested previously, then risk could potentially be mitigated, while still realizing the same cost savings since essentially the same amount of air would be added, just distributed differently.

CONCLUSIONS AND PERPESCTIVES

The integrated mathematical / knowledge-based risk assessment modelling concept by Comas et al. (2008) has been adapted for assessing the risk of N_2O production in WWTPs. The qualitative N_2O risk model approach was used to interpret mathematical simulation data and distinguish risk of N_2O production resulting from two different aeration control strategies. The approach demonstrated potential for assessing risk of N_2O production on a plant-wide level, as well as the reactor level, which allowed diagnosing specific risks and identifying opportunities for mitigation. Results also demonstrated how the N_2O risk model tool can complement the application of mechanistic models of N_2O production through the implication of specific N_2O production pathways in the risk diagnosis, which can then be used in hypothesizing underlying mechanisms and selecting appropriate mechanistic N_2O production models. The N_2O risk assessment model can also serve as a practical decision support tool for qualitatively assessing multi-criteria control strategies as seen in the results. As the Excel version of the risk assessment model was used in this study, the results not only demonstrate the potential application of the tool with mathematical model output data, but also with online, or SCADA data for operators interested in making use of the available knowledge and examining risk of N_2O production for current and historical plant operations. Work is ongoing confirming AOR values/risk and to test the entire knowledge base with full-scale data from various measurement campaigns.

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Table 1. Portion of N_2O production risk knoweldge base included in N_2O risk assessment model

Process/ Condition	Operational Parameter / Condition	ASM Variable		Risk Classification Low	Medium	High	Mechanism	References for Operational Risk Parameter Identification	References for Parameter Values
Denitrification	high NO_2	NO_2	range	<0.2	0.2 - 0.5	>0.5	- Heterotrophic denitrification - AOB denitrification	Kampschreur et al. 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011	GWRC, 2011
			units		mg/L				
Nitrification	high NO_2	NO2	range	<0.2	0.2 - 0.5	>0.5	AOB denitrification	Kampschreur et al. 2009; Foley et al., 2010; Ahn et al., 2010; GWRC, 2011	GWRC, 2011
			units		mg/L				
	low DO	DO	range	> 1.5	0.4 - 1.5	< 0.4	AOB denitrification	Kampschreur et al. 2010	Tallec et al., 2008
			units		mg/L				
	Non-limiting DO, NH4, AOR	DO	range	< 1.8	2.15	> 2.5	AOB nitrification	Ahn et al., 2010, Chandran et al., 2011, Law et al., 2012	Law et al., 2012
			units		O2 mg/L				

Table 2. Summary of overall N_2O risk results

	ASU1		ASU2		ASU3		ASU4		ASU5		Overall	
	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk	Average Overall Risk	% of Time Under High Risk
Scenario 1_DO2	0.58	21	0.31	21	0.56	33	0.41	10	0.51	19	**0.47**	**64**
Scenario 2_DO1.3	0.44	13	0.11	2.4	0.74	50	0.46	30	0.95	96	**0.54**	**98**

Table 3. Summary of Scenario Benchmarking Results

	Scenario1 DO_2	**Scenario2 DO_1.3**
Time Under High N_2O Risk (%)	64	98
Average Overall N_2O Risk Score	0.47	0.54
EQI (kg poll·d^{-1})	5612	5694
OCI (-)	10537	10023

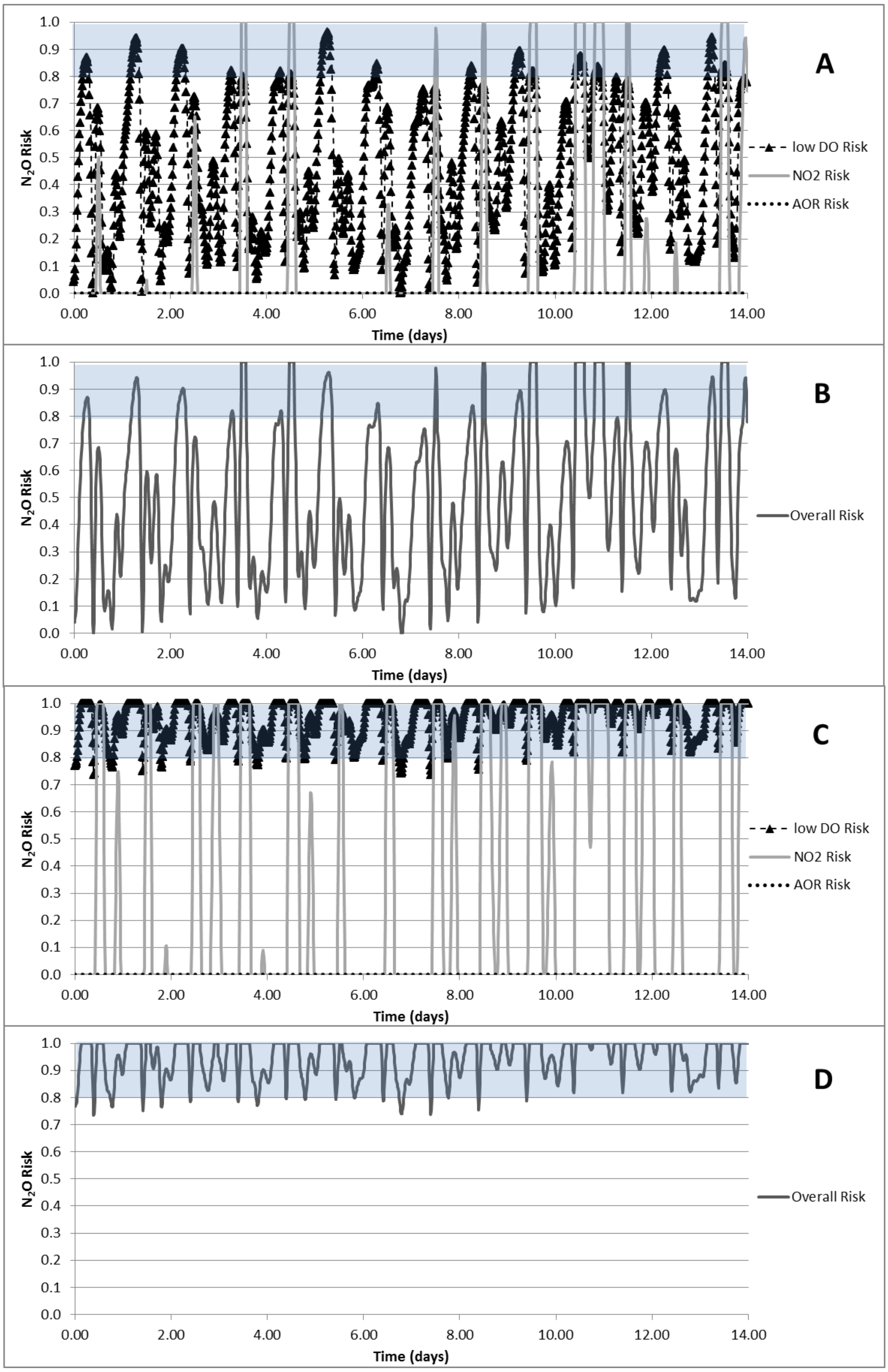

Figure 1 Dynamic N_2O risk results for ASU5: Scenario 1_DO2 individual (A) and overall (B) risks, and Scenario 2_DO1.3 individual (C) and overall (D) risks. High risk (≥ 0.8) is shaded in grey.

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