Towards a benchmarking tool for minimizing wastewater utility greenhouse gas footprints

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ABSTRACT

A benchmark simulation model, which includes a wastewater treatment plant (WWTP)-wide model and a rising main sewer model, is proposed for testing mitigation strategies to reduce the system's greenhouse gas (GHG) emissions. The sewer model was run to predict methane emissions, and its output was used as the WWTP model input. An activated sludge model for GHG (ASMG) was used to describe nitrous oxide (N_2O) generation and release in activated sludge process. N_2O production through both heterotrophic and autotrophic pathways was included. Other GHG emissions were estimated using empirical relationships. Different scenarios were evaluated comparing GHG emissions, effluent quality and energy consumption. Aeration control played a clear role in N_2O emissions, through concentrations and distributions of dissolved oxygen (DO) along the length of the bioreactor. The average value of N_2O emission under dynamic influent cannot be simulated by a steady-state model subjected to a similar influent quality, stressing the importance of dynamic simulation and control. As the GHG models have yet to be validated, these results carry a degree of uncertainty; however, they fulfilled the objective of this study, i.e. to demonstrate the potential of a dynamic system-wide modelling and benchmarking approach for balancing water quality, operational costs and GHG emissions.

Key words | benchmarking, control, dynamic modelling, greenhouse gas

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INTRODUCTION

In light of increasing voluntary and regulatory pressure on wastewater utilities to reduce their greenhouse gas (GHG) footprints, the IWA Task Group GHG is tracking and communicating ongoing efforts and proposing research directions on GHG emissions of wastewater systems. These efforts comprise both research into the source of wastewater carbon dioxide (CO_2), nitrous oxide (N_2O) and methane (CH_4) emissions and model development for use in model-based optimization and control.

Methane in collection systems

CH_4 emissions from sewers can make a significant contribution to the overall wastewater utility GHG emissions (Foley *et al.* 2009), and it is important to understand the GHG emissions from sewers for reporting accurate emissions inventories of wastewater utilities. In addition, methanogenesis within sewers has been seen to reduce wastewater chemical oxygen demand (COD) significantly

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(Guisasola *et al.* 2008), which can have a significant impact on both nutrient removal performance and N_2O production at the treatment plant. Given the complexity of sewer networks and the dynamic nature of sewer flows, modelling is an effective tool/methodology to quantify CH_4 emissions from sewers. Researchers have made some strides in modelling CH_4 emissions from pressurized sewer systems (Foley *et al.* 2009; Guisasola *et al.* 2009); however, research is required to extend current models for predicting CH_4 emissions from gravity systems as well.

Nitrous oxide

The motivation for studying N_2O emissions is that the Intergovernmental Panel on Climate Change (IPCC) (1995) reported that the global warming potential (GWP) of N_2O is 300 in CO_2 equivalents for a 100-year time horizon and N_2O is produced during the nitrogen removal process of the wastewater treatment plants (WWTPs). According to the reports of the U.S. Environmental Protection Agency (U.S. EPA 2011) and the Electric Power Research Institute (EPRI 2002), the CH_4 and N_2O emissions from WWTP account for about 0.4% and the electricity consumption makes up about 1.3% of the total national GHG emission. However, the N_2O emission is calculated following the method proposed by IPCC (2006) which can underestimate N_2O emissions (Ahn *et al.* 2010; Foley *et al.* 2010) as it is based on generic emission factors and not based on specific processes and mechanisms. This also inspires the research on N_2O production of WWTPs.

Recent research has shed light into the mechanisms/conditions leading to N_2O emissions (Kampschreur *et al.* 2008; Ahn *et al.* 2010; Yu *et al.* 2010a; Schneider *et al.* 2011). Some of this knowledge has been or is currently being translated into mathematical models that can extend existing process models to include GHG-related state variables. The common knowledge is that N_2O is an intermediate product of the heterotrophic denitrification and that the activated sludge model-nitrogen (ASMN) (Hiatt & Grady 2008) is able to simulate such processes. This model is an extension of ASM1 with two-step nitrification and four-step denitrification for modelling sequential reduction of nitrate (NO_3^-) to nitrogen gas (N_2) via nitrite (NO_2^-), nitric oxide (NO) and N_2O. However, more recently, studies have shown that NO or N_2O can also be attributed to ammonia oxidizing bacteria (AOB) under certain conditions (Colliver & Stephenson 2000; Kampschreur *et al.* 2008; Yu *et al.* 2010a) and the AOB pathway N_2O models (Kampschreur *et al.* 2007; Yu *et al.* 2010b; Houweling *et al.* 2011; Mampaey *et al.* 2011; Ni *et al.* 2011) provide meaningful representations of AOB N_2O production mechanisms to consider in efforts to build consensus and arrive at a unified model (Porro *et al.* 2012).

Corominas *et al.* (2010) implemented the ASMN (Hiatt & Grady 2008) in the framework of BSM2 (Nopens *et al.* 2010) to add N_2O production and a GHG component to the benchmarking criteria. Following this example, the authors built an activated sludge model for GHG (ASMG) which integrates N_2O production models for both AOB and heterotrophic pathways. As the N_2O pathway models are evolving, a preliminary interpretation of how they can be integrated is presented in this paper strictly to demonstrate how different solutions for mechanistic N_2O production under various process control schemes can be benchmarked. Furthermore, the framework through which new model structures can be implemented and tested as they evolve is highlighted.

GHG emissions from rivers

Once discharged, WWTP effluents can also lead to N_2O emissions in receiving waters and IPCC (2006) provides emission factors for estimating them. Moreover, river sediments can have aerobic, anoxic and anaerobic zones as its thickness increases. Therefore, denitrification and methanogenesis may occur, leading to the release of N_2O and CH_4. However, water quality models have yet to be extended to include N_2O and CH_4 production.

CO_2 and overall GHG footprint

It is critical to consider how control strategies to minimize N_2O emissions can potentially impact the overall GHG footprint and vice versa as operational strategies will likely also have an effect on energy consumption too. Methane production in sewers and through anaerobic digestion will also have a significant impact on direct and indirect CO_2 emissions. Therefore, it will be critical to understand all the interactions and transformations from a system-wide standpoint in order to properly balance GHG emissions, energy consumption/production, operating costs, and effluent water quality. However, there currently are no system-wide models available to help achieve this holistic balance, which required research on model integration for GHG purposes.

Figure 1 is a schematic of the major system-wide (i.e. collection system, treatment plant, and river) and plant-wide interactions described above and the models required for

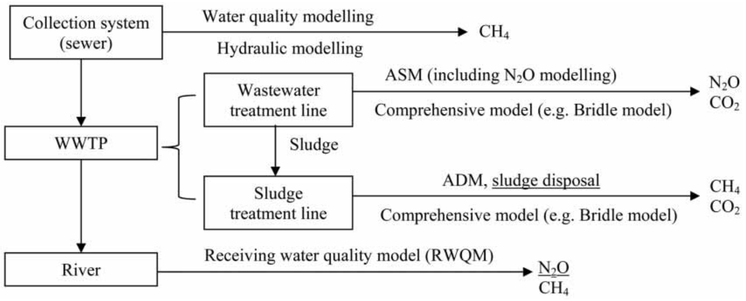

Figure 1 | System-wide GHG modelling schematic.

predicting GHG emissions. This paper discusses GHG emissions from the collection system and WWTP. It summarizes the results of the Task Group's first steps in developing a benchmark for testing mitigation strategies of urban water systems, by extending the current plant-wide benchmark (BSM2) (Jeppsson *et al.* 2007; Nopens *et al.* 2010; Flores-Alsina *et al.* 2011) to include N_2O production from autotrophic and heterotrophic pathways, and coupling it to a detailed model for CH_4 emissions from sewers based on Guisasola *et al.* (2009). The integrated model proposed in this paper provides a basis for further study on how system-wide control strategies can be developed to mitigate GHG emissions, and provides a platform including GHG emissions from receiving waters within a system-wide modelling framework. Modelling within a system-wide framework, as described in this paper, will have significant advantages over the current use of generic emission factors to estimate CO_2 and non-CO_2 GHG emissions from wastewater systems, as it can account for dynamic and mechanistic GHG production.

METHODS

The models shown in Figure 1 use very similar state variables and input parameters representing the characteristics of the wastewater. The interfaces between the models could, therefore, be conveniently developed. However, certain assumptions were made while estimating and transforming the concentrations of different COD fractions from one model to another. A detailed description of the assumptions made for linking the sewer model with the WWTP model is given in Sharma *et al.* (2012). Nopens *et al.* (2009) proposed an interface model between ASM1 and ADM1; therefore, this paper made modifications to address the new ASMG variables compared with those of ASM1. The interface from the WWTP to the receiving water bodies was not included because the rivers were not yet integrated in the system model at this stage.

Modelling of CH_4 formation in the sewer and plant interaction

For the sewer system, the model of Guisasola *et al.* (2009) was used to predict methane production in rising mains. This model adds methanogenic activity (hydrogenotrophic and acetoclastic methanogenesis) to the sewer model presented in Sharma *et al.* (2008), which describes hydrogen sulfide formation and aerobic and anaerobic carbon conversions in sewers. The model has been verified with both laboratory results and field data collected from a number of pressure mains. A network used for this study consists of pressure mains with diameters varying from 150 to 600 mm. The 150 mm mains collect sewage from gravity sewers, while the 300 mm mains collect sewage from three 150 mm pressure mains, and 600 mm mains collect sewage from 300 mm mains. To form a realistic network, three identical catchments consisting of such mains are assumed to feed the WWTP. The network is shown in Figure 2.

As the sewer model is currently not implemented in the same software platform as that for the benchmark WWTP model, its integration with the WWTP model was achieved through manual transfer. The parameters of the sewer network model were adjusted in order to produce an influent with approximately the same flow and load dynamics as the default BSM2 influent (subject to temperature variations and a typical rain series, Gernaey *et al.* 2011). The model reflected the same dynamic influent patterns as the default BSM2 influent with respect to both the flow and wastewater composition.

The sewer model was developed and implemented as described below:

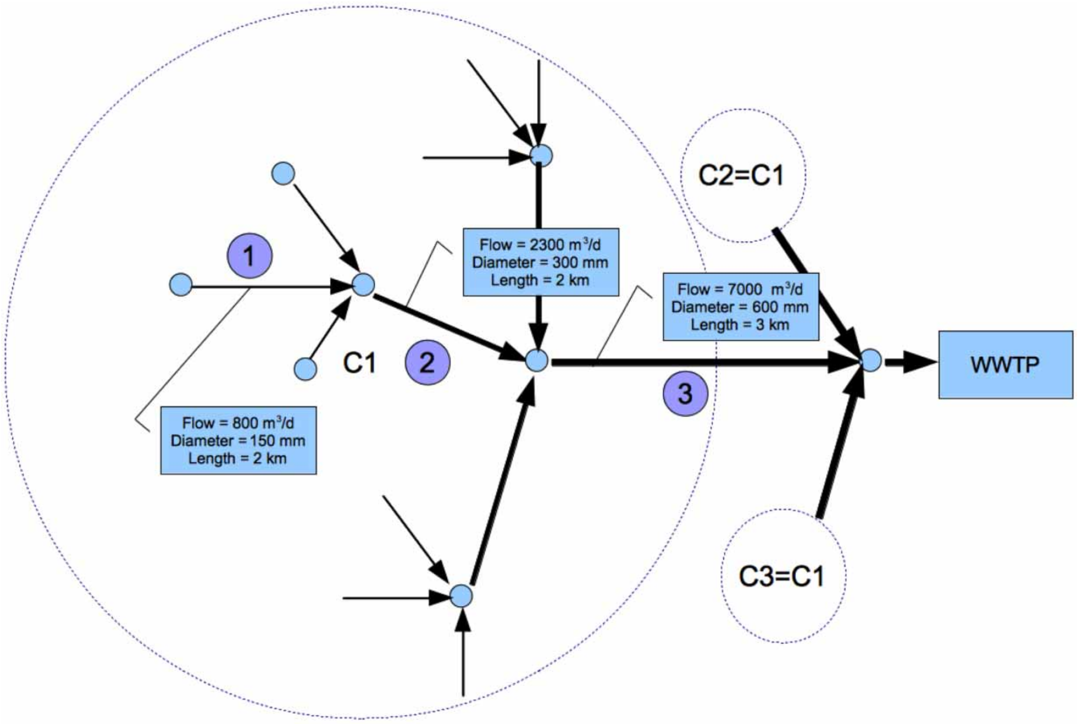

Figure 2 | Modelled sewer network.

1. The flow in each of the three catchments was obtained by dividing the total flow used in BSM2 by 3, which is 7,000 m^3/day. Each of the catchments was subdivided into three sub-catchments each carrying a flow of 2,300 m^3/day. The sub-catchment was further subdivided into three smaller catchments with a flow of 800 m^3/day each. A typical diurnal variation of wastewater flow was used (the minimum and maximum flow being 0.37 and 1.55 times the average daily flow, respectively). The flow used in the simulation included seasonal variation in the flow as well as periodic rain events.
2. The flow velocity in each of the pressure mains was calculated by dividing the flow rate by the cross-section area of the pipe. The average hydraulic retention time (HRT) in the sewer system was 5.5 h.
3. The sewer network did not have any combined sewer outflows and, for the purposes of this paper, detailed hydraulic components, such as headloss, tailwater effects and flow routing, were not considered. However, detailed hydraulics can be included in future studies to examine how this effects various sewer design and hydraulic conditions and can impact CH_4 production and emissions.
4. In order to simulate plug flow in the pressure main sewers, each sewer section was divided into a number of completely mixed reactors connected in series. Biochemical reactions in each of the tanks together with the connective transport were considered in the model.
5. The BSM2 influent was used as the reference output of the sewer model. As such, the raw wastewater characteristics were adjusted to arrive at a wastewater composition similar to the BSM2 influent at the end of the pipe. As the objective of sewer modelling herein was to find out the levels of methane produced in sewers for the wastewater with the same characteristics as the BSM2 influent being discharged at the end of the sewer, this methodology was deemed sufficient for the purpose of this study.
6. The sewer system was simulated for 609 days and CH_4 production was calculated over the last 364 days. It was assumed that all of the dissolved CH_4 produced in the model is transferred to the gas phase at the sewer outlet/plant influent, where there is typically a significant amount of turbulence and mixing, leading to ideal stripping conditions. Actual liquid-to-gas mass transfer coefficients in the open environments should be investigated further as indicated by Foley *et al.* (2009). Moreover, the GHG emissions related to energy, mainly for pumping, are not included in the current paper and should be a subject of further studies.

Modelling of N_2O emissions from WWTP

As the basis of the WWTP model, the BSM2 modelling platform (Nopens *et al.* 2010) was used to predict plant-wide GHG emissions, Figure 3. The activated sludge process is a modified Ludzack–Ettinger (MLE) process. It consists of five activated sludge units (ASUs) in series. ASU1 and ASU2 are anoxic, while ASU3, ASU4 and ASU5 are aerobic.

The ASMG is proposed as bio-kinetic model for the activated sludge, considering N_2O production by both heterotrophic and AOB denitrification, and implemented in the BSM2 modelling platform. The model combines ASMN for the heterotrophic N_2O production pathway and an AOB denitrification model for the AOB pathway. However, the AOB denitrification models are still under discussion (Kampschreur *et al.* 2007; Yu *et al.* 2010b; Mampaey *et al.* 2011; Ni *et al.* 2011). The key differences between these models are with regard to NO and N_2O pathways, and what role dissolved oxygen (DO) concentration plays in AOB denitrification. However, this is not the focus of this paper whose main purpose is to demonstrate the usefulness of a benchmark tool for assessing the overall carbon footprint of wastewater systems, and how N_2O and CH_4 models can be critical components of the tool. A model based on Scenario A, i.e. the aerobic scenario, of Mampaey *et al.* (2011) was implemented. The NO_2^- and NO reduction use electrons from the ammonia oxidation. The same concept was used in the AOB denitrification model of Kampschreur *et al.* (2007). Two modifications were done to Scenario A of Mampaey *et al.* (2011): the growth correction factor to the AOB denitrification, and changing the DO inhibition term as a competitive term. The modified kinetic equation for AOB denitrification is as Equation (1):

$$r_{\mathrm{AOBden.}} = \mu_{\mathrm{AOB}} \cdot \eta_{\mathrm{AOB}} \cdot \frac{K_{\mathrm{comp}} \cdot S_{\mathrm{O}}}{K_{\mathrm{SO\_mod.AOB\,den.}} + S_{\mathrm{O}} + S_{\mathrm{O}}^2/K_{\mathrm{IO\_mod.AOB\,den.}}} \cdot \mathrm{A} \qquad (1)$$

where A is a multiplication term of X_{AOB} and the inhibition terms of NO_2^- (or NO) and ammonia, μ_{AOB} is the maximum growth rate (d^{-1}), η_{AOB} is the growth correction factor for AOB denitrification, and K_{comp}, $K_{\mathrm{SO\_mod.AOBden.}}$ and $K_{\mathrm{IO\_mod.AOBden.}}$ are the parameters which can be calculated from the half-saturation DO concentrations, Equations (2)–(4):

$$K_{\mathrm{comp}} = \frac{1}{1 - 2 \cdot \sqrt{K_{\mathrm{SO\_mod.AOB\,den.}}/K_{\mathrm{IO\_mod.AOB\,den.}}}} \qquad (2)$$

$$K_{\mathrm{SO\_mod.AOB\,den.}} = \frac{S_1 \cdot S_2}{K_{\mathrm{IO\_mod.AOB\,den.}}} \qquad (3)$$

$$K_{\mathrm{IO\_mod.AOB\,den.}} = \frac{\left(\sqrt{S_1} - \sqrt{S_2}\right)^2}{K_{\mathrm{comp}}} \qquad (4)$$

where S_1 and S_2 are the half-saturation DO concentrations (mg/l).

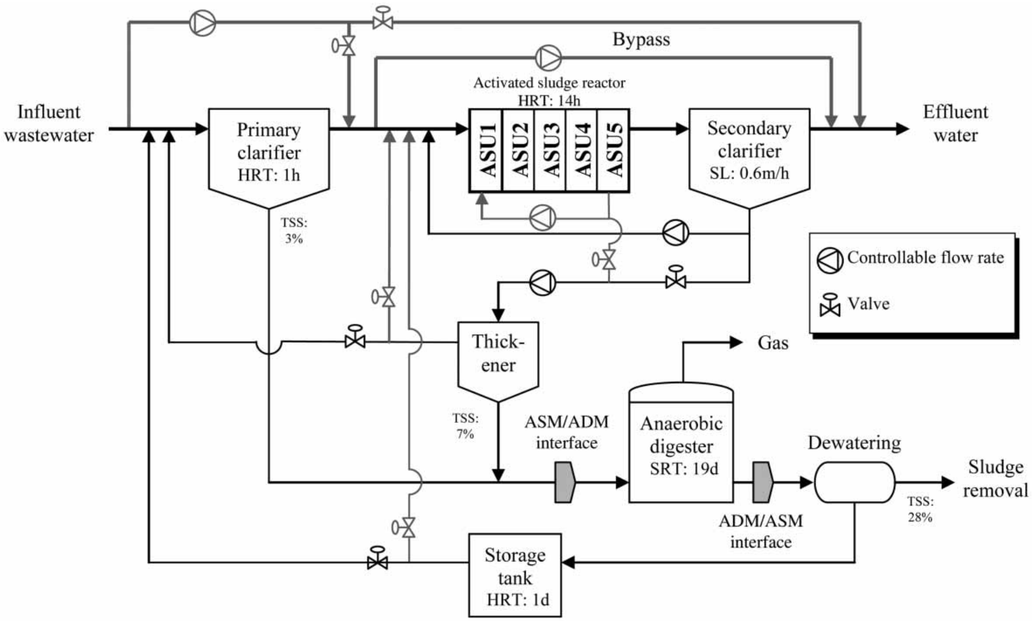

Figure 3 | BSM2 plant configuration (Nopens *et al.* 2010).

Gas stripping equations for calculating the gas emission rates are also included. The interfaces between ASMG and ADM1 followed the method proposed by Nopens *et al.* (2009) for transferring components between ASM1 and ADM1 models, except that the new components that were added in ASMG, i.e. NO_3^-, NO_2^-, NO, N_2O, N_2, AOB and NOB, and the mapping of COD and N was adjusted accordingly. The four oxygen providing N-species NO_3^-, NO_2^-, NO and N_2O were considered in the ASMG-ADM1 interface (transferring ASMG components to ADM1) while AOB and NOB were used to provide COD for denitrification at the interface. With their complete removal, AOB and NOB also contributed to the nitrogen input of the interface. Also, NO_3^- and NO_2^- were taken into account for charge balance. For the ADM1-ASMG interface, the concentrations of all new components were assumed to be 0 mg/l. The same interfaces were used by Flores-Alsina *et al.* (2011).

Parameter adjustments were required because individually the ASMN and AOB denitrification models account for only one pathway of N_2O production. When the two models were combined, the model structure was different from their individual models which required parameters to be recalibrated. Moreover, ASMN was developed for high strength wastewater treatment (Flores-Alsina *et al.* 2011) and Mampaey *et al.* (2011) had not implemented their model in a plant-wide activated sludge system. The model parameters were adjusted using the open loop ASM1–BSM2 (Nopens *et al.* 2010) results as reference, with three objectives: the N_2O emission factor, the effluent quality and the operational cost. The reported N_2O emission factor in the literature is usually in the range of 0.1–1% of the influent total nitrogen (TN) load for plants with a MLE process (Ahn *et al.* 2010; Foley *et al.* 2010). BSM2 is also a MLE plant. Therefore, 0.5% was chosen as the N_2O emission factor for model parameter adjustment. Effluent quality, including the Effluent Quality Index (EQI) and the average effluent concentrations, and Operational Cost Index (OCI) should also agree with the results given in the finalized ASM1–BSM2 (Nopens *et al.* 2010). The adjusted parameters of ASMG that satisfy these three criteria are given in Table 1.

The simulations included a steady-state simulation followed by a dynamic simulation of 609 days. Only the data generated during the last 364 days of the dynamic simulation (starting on 1 July) are used for plant performance evaluation.

Effluent quality, operational cost and GHG indices

The plant-wide performance is evaluated by the EQI, the OCI and by the GHG emissions index. EQI and OCI were calculated using the BSM2 methodology (Nopens *et al.* 2010). The overall GHG emissions from the treatment plant, quantified as CO_2 equivalents followed the method proposed by Corominas *et al.* (2010) and used by Flores-Alsina *et al.* (2011). This GHG evaluation method uses the N_2O emissions directly from the integrated bioreaction model and estimates other GHGs by processing the results of ASMG using the Bridle model (Bridle *et al.* 2008), which uses empirical relations to calculate the GHG emissions due to CO_2 from biotreatment, CH_4 from anaerobic digestion, power consumption and carbon dosing.

Scenario analysis

To examine the overall behaviour of the N_2O models and the relative impact of different control strategies, scenarios concerning the ratio of COD and nitrogen source (COD/N ratio), DO and cascade control were investigated as listed in Table 2.

Open loop kept Kla at constants and studied the effect of different external carbon dosing rate. The open loop with external carbon dosing of 2 m^3/d was taken as the default scenario. Scenario 1 and 2 controlled DO concentrations in aerobic tanks. Scenario 1 used a single DO controller, i.e. controlling DO of ASU4 by manipulating Kla3-5 in ratios, while Scenario 2 used two DO controllers, i.e. controlling DO of ASU3 independently from ASU4-5. The final scenario was a cascade control which tried to maintain ammonia concentration of ASU5 by adjusting Kla3-5. The cascade control strategy adds a minimal DO concentration requirement for the first aerobic tank ASU3. The purpose of the cascade control is to limit the ammonia violation with minimal aeration energy consumption. Hence, in some cases when the effluent ammonia concentration is low, the controller will allow the DO to drop to low values. The resulting low DO concentrations can result in high NO_2^- concentrations and then promote the N_2O production by AOB. In order to make the N_2O production not substantially exceed other control strategies, the DO of ASU3 is kept above 1 mg/l in the cascade control. In other words, the DO controller of ASU3 receives two signals for Kla3: one being a ratio to the Kla5 and the other imposing a minimal DO concentration. The controller picks the larger

Table 1 | Adjusted parameters of ASMN and AOB denitrification model

Parameter	Unit	Suggested value in respective reference	Adjusted value
ASMN			
b_{AOB}	d^{-1}	0.096	0.048
b_{NOB}	d^{-1}	0.096	0.048
b_H	d^{-1}	0.408	0.53
k_a	l/(mg biomass COD d)	0.1608	0.1
K_{FA}	mg N/l	0.0075	0.004
K_{FNA}	mg N/l	0.0001	10^{-6}
k_h	mg COD/(mg biomass COD d)	2.208	5
K_{I10FA}	mg N/l	0.2	0.5
K_{I10FNA}	mg N/l	0.04	0.1
K_{I5NO}	mg N/l	0.075	0.2
K_{N2O}	mg N/l	0.05	0.02
K_{NO}	mg N/l	0.05	0.04
K_{NO2}	mg N/l	0.2	0.3
K_{NO3}	mg N/l	0.2	1.5
K_{OH}	mg COD/l	0.1	0.2
K_{OH1}	mg COD/l	0.1	0.2
K_{OH2}	mg COD/l	0.1	0.2
K_{OH3}	mg COD/l	0.1	0.2
K_{OH4}	mg COD/l	0.1	0.2
K_{OH5}	mg COD/l	0.1	0.2
K_{S1}	mg COD/l	20	15
K_{S5}	mg COD/l	40	30
K_X	mg COD/mg biomass COD	0.15	0.1
η_{g2}	–	0.28	0.3
η_{g3}	–	0.16	0.3
η_{g4}	–	0.35	0.6
η_{g5}	–	0.35	0.8
η_h	–	0.4	0.8
Y_H	mg biomass COD formed/mg N removed	0.6	0.67
AOB denitrification model			
$K_{NO2\_AOBden.}$	mg N/l	8	2
$K_{SO\_AOBden.}$	mg COD/l	0.5	–
$K_{SO\_mod.AOBden.}$	mg COD/l	–	11.40
$K_{IO\_mod.AOBden.}$	mg COD/l	–	0.035
η_{AOB}	–	1	0.5

Note: the reference temperature is 20°C; the ASMN suggested values are from the paper by Hiatt & Grady (2008); the suggested values for the AOB denitrification model are from Mampaey *et al.* (2011).

value for Kla3. These control strategies were selected as they are increasingly used in WWTPs and could reflect the response to the increasing pressure of reducing energy and CO_2 emissions.

RESULTS AND DISCUSSION

One must be aware that the results shown herein may not be completely representative of potential system-wide GHG

Table 2 | Scenarios tested in this paper

Open loop (COD/N ratio)	Q_carbon $= 2\ \text{m}^3/\text{d}$ (default) Q_carbon $= 4\ \text{m}^3/\text{d}$	$\text{Kla3} = 1.5{\cdot}\text{Kla4} = 3{\cdot}\text{Kla5} = 210\ \text{d}^{-1}$
Scenario 1 (1 DO control)	DO_SP4 = 2 mg/l DO_SP4 = 1.5 mg/l	$\text{Kla3} = 1.5{\cdot}\text{Kla4} = 3{\cdot}\text{Kla5}$
Scenario 2 (2 DO control)	DO_SP3 = 2.0 mg/l DO_SP4 = 1.0 mg/l DO_SP3 = 1.0 mg/l DO_SP4 = 2.0 mg/l	$\text{Kla4} = 2{\cdot}\text{Kla5}$
Scenario 3 (NH_4^+-DO cascade control)	NH_4^+_SP5 = 1.0 mg/l DO_SP5 = NH_4^+_u5 DO_Min3 = 1.0 mg/l	$\text{Kla3} = 1.5{\cdot}\text{Kla4} = 3{\cdot}\text{Kla5}$

Note: Q_carbon, carbon dosing flow rate (the carbon dosing concentration is 400 kg COD/m^3); Kla3-5, oxygen transfer coefficients in ASU3-5; DO_SP3-5, DO set points of ASU3-5; NH_4^+_SP5, NH_4^+ set point in ASU5; NH_4^+ _u5, output of NH_4^+ controller in ASU5; DO_Min3, the minimum DO requirement of ASU3; the external carbon dosing flow rate in the Scenario 1–3 is the same as the default 2 m^3/d.

emissions for the given conditions, as the N_2O models are still under development. The changes seen in simulation values with changing models and their parameters, particularly with the AOB denitrification pathway model, are still not fully understood as consensus on AOB pathways is yet to be reached. A lot of factors affect N_2O production and one single change (either increase or decrease) of a factor can give rise to two opposite effects. This paper should therefore not be used for interpretation of the underlying mechanisms.

Rather, the results are intended to illustrate the potential of building a system-wide benchmark for GHG emissions modelling and control, and shows how the interaction between sewers and WWTPs and the various factors affecting GHG emissions can be studied. The framework is now in place and can easily be rerun as model structures evolve, parameter adjustments become necessary, and to test/compare different models.

CH_4 emissions from the collection system

Similar to BSM2, the methane production was calculated over the last 364 days of 609-day dynamic simulation, i.e. from Day 245 to Day 609. This evaluation period starts in summer and after 364 days ends in summer again. Day 245 corresponds to 1 July and Day 609 to 30 June. The highest temperature in summer is about 20 °C and the lowest temperature in winter is about 10 °C. After July and August when the temperature is around 20 °C, the temperature begins to decrease and reaches about 15 °C in November. The temperature further decreases to 10 °C at the end of February and then it starts warming up to 15 °C in June.

Over the last 364 days, the average methane production in the sewer was 60.2 kg CH_4/day, which gives an annual methane production of 21.9 tons. Figure 4 shows the variation of the methane produced in the sewers and released at the outlet, indicating the methane concentration can vary significantly under the imposed dynamic conditions, including rain events. The variation in methane concentration is due to flow rate and temperature. The flow rate shows impacts mainly on diurnal variation (short-term fluctuation), while the temperature is the major factor for seasonal variation (long-term variation) of methane concentration. The flow rate affects HRT and therefore influences the methane production. Two types of flow variations were considered: (1) diurnal flow variation; and (2) flow increase during rainfall events, which reached a level three to four times the average flow rate. The seasonal variation of temperature is shown to have impacts on methane production, as higher temperature results in higher

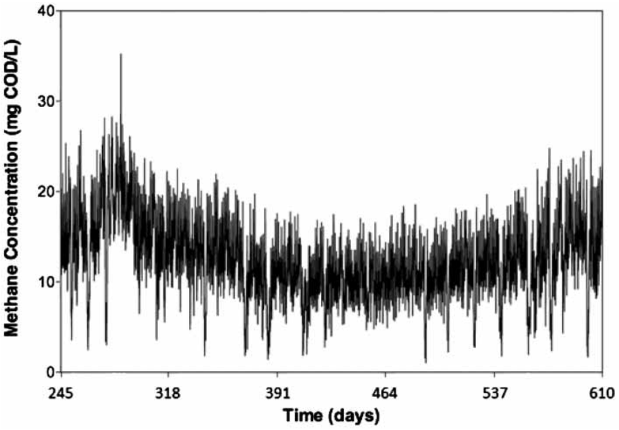

Figure 4 | Emitted methane concentration at sewer outlet.

biological activity in sewer biofilm. It is clearly shown in Figure 4 that methane concentration is higher in summer than in winter, reaching a maximum of 35 mg COD/l in summer. Seasonal variation in wastewater flow rate may also add to this variation, but the contribution is expected to be smaller compared with that of temperature variation.

The methane production variation highlights the importance of modelling the system dynamically to understand the potential GHG emission from sewers and points to the need for better understanding CH_4 formation in sewers in relation to treatment plant performance, and the plant N_2O emissions potential based upon influent COD/nitrogen ratios. It should be noted that the production of methane in sewers depends upon the characteristics of sewer networks such as the type of sewer (gravity or pressure main), length of sewer pipe, pipe diameter, HRT and temperature. Any changes to these characteristics/conditions will result in a different methane production rate, which could be a noteworthy disadvantage to designing bigger sewers than necessary as detention times and methane production would increase.

N_2O and total GHG emissions from WWTP

Figure 5 summarizes the averaged results for the dynamic simulations using the plant-wide extended BSM2 model. The N_2O equivalents were calculated by multiplying the N_2O gas emission rate with the N_2O's GWP value 300 (IPCC 1995). For the scenarios analysed in the current paper, the amount of methane emissions from the sewers contributes around 6–7% of the total sewer-plant system GHG emissions, while the total emission from biotreatment makes up the largest component of the total net WWTP emissions, around 43–52%, which includes the CO_2 generated from biomass respiration and BOD oxidation, the N_2O generated from nitrogen removal, and the CO_2 credit from nitrification. Among the different categories of GHG emissions from biotreatment, N_2O represents 4–16% of the total net sewer-plant system emissions. The GHG emissions under the heading 'Other' are almost the same for all scenarios, which includes the contributions from the digester, sludge reuse and other energy consumptions. The different scenarios also show a great similarity in terms of Aeration, Power credits and Chemical use. Therefore, N_2O plays a major role in differentiating the total WWTP GHG emissions.

For all scenarios, including the open loop and the control strategies, the average N_2O liquid concentrations in the ASUs are below 0.001 mg/l, so it can be deduced that the average effluent N_2O concentration will also be less than 0.001 mg/l. The average effluent flow rate over the last 364 days is 21,014 m^3/d, so the average N_2O flux rate discharged with plant effluent is about 21 g N_2O-N/d. The average N_2O stripping rate of the activated sludge reactor is 5.15 kg N_2O-N/d. Therefore, the N_2O discharged with plant effluent accounts for a negligible fraction of the GHG emissions compared with other emissions of WWTP GHG.

Effect of COD/N ratio – open loop

As can be seen from Figure 5, increasing the carbon addition slightly decreases the overall N_2O emission. However, this trend is not absolute. Carbon dosing benefits the heterotrophic denitrification when the influent carbon source is insufficient, and then may reduce the heterotrophic N_2O production. However, the DO concentrations in the aerobic tanks with more carbon dosed may be lower, because more residual organics can flow into the aerobic tank leading to more oxygen consumption; the lower DO concentration can subsequently cause a higher

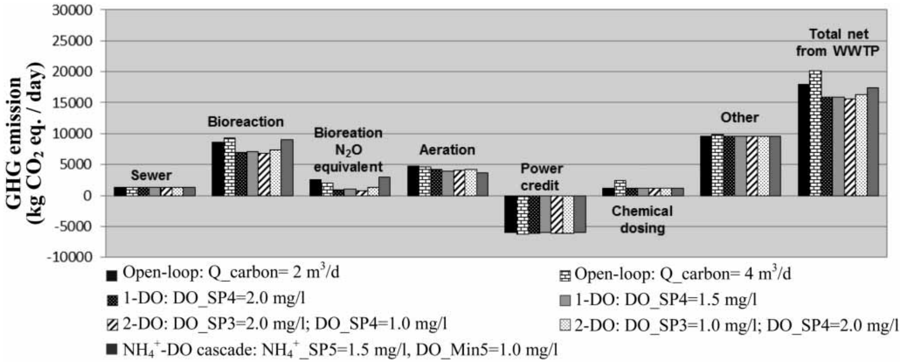

Figure 5 | Daily averaged GHG emissions summary for evaluated scenarios (Q_carbon: carbon dosing flow rate; DO_SP3: DO set point of ASU3; DO_SP4: DO set point of ASU4; NH_4^+_SP5: NH_4^+ set point in ASU5; DO_Min5: the minimum DO requirement of ASU5).

NO_2^- concentration and then increase N_2O production by AOB. Whether the overall N_2O production will increase or decrease depends on which pathway or direction is dominant. In this study, the reduction of heterotrophic N_2O production dominated and gave the lower N_2O emission under the higher carbon dosing rate. Looking at the rates of N_2O net production, the N_2O net production by AOB is 5,804 gN/d under the carbon dosing rate of 2 m^3/d while it is 6,634 gN/d when the dosing rate is 4 m^3/d, which means more N_2O is produced by AOB under elevated carbon dosage. However, the N_2O total net production is 4,980 gN/d for the carbon dosing of 2 m^3/d and 3,567 gN/d for 4 m^3/d, i.e. more carbon dosing helps the heterotrophic denitrification which reduces the N_2O total net production. N_2O is denitrified by heterotrophs to N_2 and the heterotrophic N_2O net production rates were negative values, because heterotrophs also denitrify the N_2O produced by AOB.

However, the difference on N_2O emissions is not substantial compared with the difference between the different control strategies. Also, the total GHG emission due to bioreaction with more carbon dosing exceeds the default open loop, because more CO_2 is generated by BOD oxidation. The GHG emission due to chemical use is doubled when the carbon dosing flow rate is increased from 2 to 4 m^3/d. Therefore, in total, the open loop scenario with more carbon dosing emits more total net WWTP GHGs. However, in view of the total net WWTP GHG emissions, the chemical dosing only contributes by a small portion, i.e. 12% for the open loop with high carbon dosing and around 7–8% for the other scenarios. Generally speaking, the key message from this scenario is not that more carbon dosing will produce more N_2O, but to illustrate that the carbon dosing can affect the N_2O production. However, it is shown that such effect is not substantial and that the GHG production from the carbon dosing is a minor one compared with the bioreaction.

As mentioned previously, each scenario was simulated under steady-state and dynamic conditions. This was done to assess the implications of using steady-state models or emission factors to describe N_2O emissions, which have been seen to vary substantially under dynamic conditions (Kampschreur *et al.* 2008; Yu *et al.* 2010a). The default open loop case was looked at in particular. Figure 6 compares the N_2O emissions under steady-state and dynamic conditions for the default open loop. Although the Influent Quality Index (IQI) of the last 364 days for steady-state and dynamic influent are very similar, 74,746 and 74,785 pollution units/d respectively, the two cases show a very significant difference in N_2O emissions (note the difference in vertical axes of Figure 6). Under steady-state conditions, the N_2O emission rate is only 1.08 kg N_2O-N/d, while the value averaged for the last 364 days of dynamic simulation is 5.15 kg N_2O-N/d with a wide range of 0.57–267.16 kg N_2O-N/d. The large fluctuation introduces difficulties to approximate the dynamic changes by steady-state simulation. This clearly highlights the need for dynamic models, as already suggested in Corominas *et al.* (2012), to accurately predict N_2O emissions and also underlines the necessity for dynamic sewer models to generate a dynamic influent. It also demonstrates the necessity to develop mitigation strategies based on dynamic conditions.

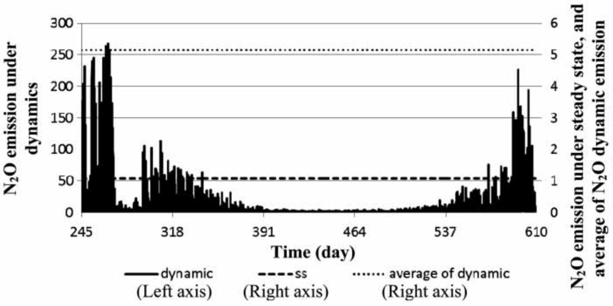

Figure 6 | Comparison of N_2O emission under the steady-state and the dynamic simulation.

Effect of DO – Scenario 1 and 2

DO is connected to N_2O emission in two ways, i.e. N_2O gas stripping through aeration which fluctuates to follow the desired DO concentration, and N_2O production related to bioreactions with DO participating. In the 1 DO control strategy, more NO_2^- could be produced under the lower DO conditions which would stimulate AOB denitrification to produce N_2O; however, on the other hand, the lower DO setpoint means a smaller aeration flow rate which strips less N_2O into the atmosphere, and the lower DO set point reduces the aeration energy consumption. One disadvantage of the 1 DO control strategy is that it cannot control the DO concentration of the aerobic tanks individually. Therefore, the spatial distribution of DO concentrations cannot be set. However, the N_2O production is heavily related to this DO distribution, as is clearly shown in the 2 DO control strategy and Figure 7 which compares the N_2O emission in each tank under the 2 DO control strategies. The 1 DO control strategy may give rise to a DO spatial profile which

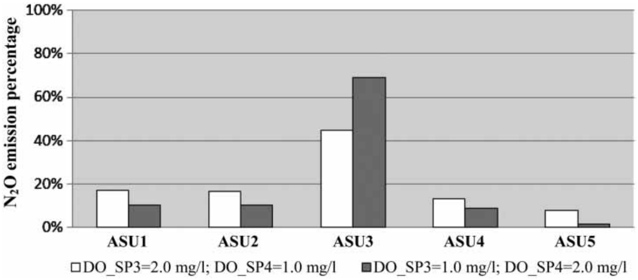

Figure 7 | N_2O emission percentages in each ASU under different 2 DO strategies.

unintentionally supports the N_2O mitigation. Consequently, the 1 DO control strategy is not specific enough for N_2O control because the DO spatial profile is unknown and may change at any time.

Under the low-high 2 DO control strategy, more N_2O is emitted in the ASU3 than under the high-low 2 DO control strategy. In the ASU3, ammonia is still present and can be used as electron donor for the AOB denitrification to produce the N_2O. The low DO concentration is beneficial for AOB denitrification and a lot of NO_2^- is produced under such a low DO setpoint. All these help N_2O production by AOB in the low-high 2 DO control strategy. Therefore, in order to limit N_2O production in ASU3, the high-low 2 DO control strategy keeps the DO concentration at a high level in the ASU3; then most of the ammonia is oxidized and little is left in ASU4 which reduces N_2O production by AOB denitrification. The results of Scenario 2 further confirm that a different DO distribution may also yield a different N_2O emission even if they have the same energy consumption due to aeration, suggesting that the effect of the spatial distribution of DO warrants further investigation, e.g. the 3 DO control strategy.

Results of cascade control – Scenario 3

By using this cascade control strategy, the overall GHG emissions show a slight improvement compared with the default open loop case and are ranked third overall, which is higher than the other control strategies, although the DO of ASU3 is set with a minimum to limit the N_2O production. The disappointing performance of the cascade strategy on the N_2O control is probably related to the fact that the original design of the cascade control is driven by the wish to (1) guarantee the effluent ammonia quality with few violations and (2) reduce the aeration energy consumption. It is not a strategy focusing on N_2O mitigation, but within this framework can be assessed in terms of its energy efficiency and net GHG emissions.

Effluent quality operational cost and GHG indices

Table 3 uses a less quantitative way to compare EQI, OCI and total net GHG emissions. The symbols '+' or '−', instead of listing digital numbers, were given to express the relative increase or decrease of each scenario compared with the default scenario.

The results show that by using closed-loop strategies, the OCI or EQI and the GHG emissions reduced more or less compared with the open-loop scenarios. As stated before, the cascade control is intentionally designed for limiting ammonia effluent violations of the wastewater biotreatment. Therefore, the largest decrease of aeration energy consumption and OCI led to a sharp drop of ammonia violations and the largest improvement on daily averaged EQI among all tested scenarios. In Scenario 2 where two kinds of DO distribution strategies are tested, the different patterns of DO

Table 3 | Daily averaged OCI, EQI and GHG of each scenario

Scenarios		OCI (energy units/d)	EQI (pollution units/d)	GHG (kg CO_2eq./day)	Ammonia violation[a] (% of total evaluation time)
Open loop	Q_carbon = 2 m^3/d (default)	Null	Null	Null	Null
	Q_carbon = 4 m^3/d	+ + +	− − −	+ + +	+ + + +
Scenario 1	DO_SP4 = 2 mg/l	−	i	− − −	− − − −
	DO_SP4 = 1.5 mg/l	− −	−	− − −	− − − −
Scenario 2	DO_SP3 = 2.0 mg/l DO_SP4 = 1.0 mg/l	− −	−	− −	− − − −
	DO_SP3 = 1.0 mg/l DO_SP4 = 2.0 mg/l	− −	−	− −	− − − −
Scenario 3	NH_4^+_SP5 = 1.0 mg/l DO_SP5 = NH_4^+_u5	− − −	− − −	−	− − − − −

Note: a, the effluent ammonia limit is set to 4 mg/l; from single to multiple '+' or '−', the relative increase or decrease is 1–5%, 5–10%, 10–50%, 50–99% and larger than 100%; 'i' means the change is below 1% and can be neglected.

distribution give different performance on GHG emissions due to the different N_2O emissions, although they have almost the same aeration energy consumption and similar OCI, which again supports the further investigation and optimization by using DO spatial distribution strategies.

The use of the BSM2 tool to evaluate scenarios in this manner clearly demonstrates the potential to evaluate various control strategies and find the right balance for a specific system, which will depend on the individual utilities' priorities.

CONCLUSIONS AND PERSPECTIVES

Initial steps in developing a system-wide modelling framework for minimizing GHG footprints of urban wastewater systems based on BSM2 were presented. A sewer and plant-wide model were used and coupled indirectly to assess the potential system-wide emissions and to evaluate various control strategies. Sewer methane emissions make a non-negligible and potentially significant contribution to the total system net GHG emissions, while WWTP N_2O emissions make a significant contribution.

For scenarios studied in the paper, the DO shows an important effect on N_2O emissions and its spatial distribution should be considered in the strategy design; the cascade control has problems with controlling N_2O emissions but makes up some ground in OCI and EQI; carbon dosing influences the N_2O production to a small extent and contributes only a small part to the total GHG when compared with the bioreaction.

The intent of this paper is not to imply findings on mechanisms or pathways, but to demonstrate the potential and construction of a system-wide modelling and benchmarking approach for balancing water quality, operational costs and GHG emissions, and to test its sensitivity to logical changes in system design and control. The development of this tool is also purposely working in parallel to the development of improved GHG models, which will actually help the progression of GHG models by allowing them to be tested as they evolve.

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