A dynamic modelling approach to evaluate GHG emissions from wastewater treatment plants

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Abstract

The widened scope for wastewater treatment plants (WWTP) to consider not only water quality and cost, but also greenhouse gas (GHG) emissions and climate change calls for new tools to evaluate operational strategies/treatment technologies. The IWA Benchmark Simulation Model no. 2 (BSM2) has been widely used within the scientific community for the unbiased comparison of control strategies in wastewater treatment facilities. In this paper, the default set of BSM models is extended with a set of comprehensive dynamic approaches that estimate the most significant on-site (secondary treatment, sludge processing) and off-site (net energy use, embedded chemicals, sludge disposal) sources of GHG emissions. The case study presented here calculates and discusses the changes in the effluent quality (EQI) and operational cost (OCI) indices and the formation of carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O) when modifying the percentage of total suspended solids (TSS) removal efficiency in the primary clarifier (PRIM). Simulations show that high PRIM efficiency decreases the quantity of TSS entering the activate sludge (AS) section leading to lower operational cost due to better energy recovery (and subsequent reduced GHG emissions) in the sludge line, but increases the overall N_2O emissions due to the low C/N ratio as a trade-off. Overloading of the bioreactors as a result of poor PRIM performance: i) increases the biogenic CO_2 emissions from BOD oxidation and biomass decay in the AS section; ii) increases off-site CO_2 emissions due to higher energy demand during the nitrification stage; and, iii) reduces energy recovery from settled organics. The reported results emphasize the importance of a plant-wide approach and the need to consider the interactions between the different treatment units when evaluating the global warming potential (GWP) of a WWTP. Finally, the paper demonstrates the potential of using the proposed approach as a general model-based tool for determining the most sustainable WWTP operational strategies, which is essential in a water sector where climate change, energy and sustainability are key challenges to be tackled.

Keywords: Activated sludge modelling, Benchmarking, Global warming, Model-based evaluation, Multi-criteria decision making, Process control, Sustainability

INTRODUCTION

The constantly changing nature of wastewater (quantity/quality), its unknown origin and the great variety of ambient conditions make wastewater treatment plants (WWTPs) truly dynamic systems. Comprehensive studies and full-scale applications (**Olsson *et al.*, 2005**) have shown the feasibility of using automatic control to optimize the operation under these conditions. WWTP models and simulation studies have been used to evaluate performance and compare control strategies in general (**Gernaey *et al*., 2012**) or before full-scale implementation (**Ayesa *et al*., 2006**). The complexity of modern WWTPs with different sub-processes, interconnections and recirculation makes it necessary to consider a plant-wide perspective in order to avoid sub-optimal performance (**Olsson and Newell., 1999; Jeppsson *et al*., 2007; Nopens *et al*., 2010**).

The main focus for a WWTP has historically been the effluent water quality under constraints of technical feasibility and cost. This is still true, but the discussion on sustainability in general, and the issue of climate change due to greenhouse gas (GHG) emissions in particular, have widened the scope for the utilities. An increasing interest for GHG emissions calls for new approaches to reach the high and increasing demands on effluent quality and at the same time predict and minimize the GHG emissions. New tools are needed to accomplish this goal.

The main objective of this paper is to demonstrate a mathematical approach to evaluate GHG emissions from WWTPs taking into account system dynamics. The authors suggest a set of models that quantify on-site (secondary treatment, sludge processing) and off-site (net energy use, embedded chemicals, sludge disposal) sources of GHG emissions. A case study is presented where changes in effluent quality, operational cost and CO_2, CH_4 and N_2O emissions are analyzed in a plant-wide fashion when the total suspended solids (TSS) removal efficiency in the primary clarifier is modified. The paper also i) includes a critical discussion of the results, ii) envisages new research needs and directions, and, iii) provides guidelines to make the tool more general and applicable to other (real) cases.

METHODS

WWTP under study

The WWTP under study (BSM2G) has the same layout as the IWA BSM2 proposed by **Jeppsson *et al*. (2007)** and **Nopens *et al*. (2010).** The activated sludge unit is a modified Ludzack-Ettinger configuration consisting of 5 tanks in series. Tanks 1 (ANOX1) and 2 (ANOX2) are anoxic, while tanks 3 (AER1), 4 (AER2) and 5 (AER3) are aerobic. AER3 and ANOX1 are linked by means of an internal recycle. The BSM2G plant further contains a primary (PRIM) and a secondary (SEC) clarifier, a sludge thickener (THK), an anaerobic digester (AD), a storage tank (ST) and a dewatering unit (DW) (see layout in **Figure 1**).

From the original set of models, the activated sludge model no 1 (ASM1) (**Henze *et al*., 2000)** has been expanded with the principles stated in **Hiatt and Grady (2008)** to take into account N_2O formation during denitrification. This model incorporates two nitrifying populations: ammonia oxidizing bacteria (AOB) and nitrite oxidizing bacteria (NOB) using free ammonia and free nitrous acid, respectively, as their substrates. The model also considers sequential reduction of nitrate to nitrogen gas via nitrite, nitric oxide and nitrous oxide using individual reaction specific parameters. Additionally, the ideas summarized in **Mampaey *et al*. (2011)** are used to consider NO and N_2O formation during the nitrification pathway assuming ammonia as the electron donor.

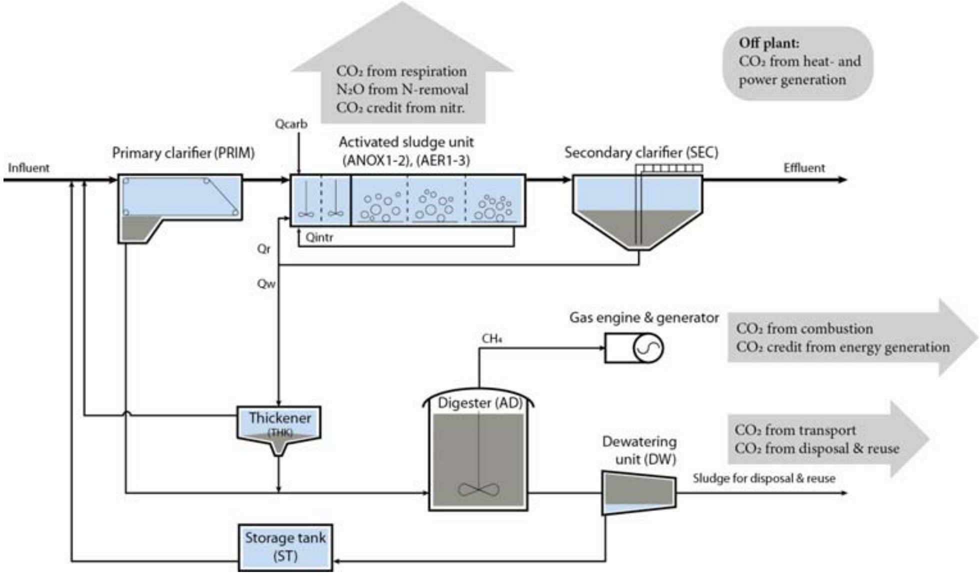

Figure 1. BSM2G plant layout including GHG sources (grey boxes).

The interfaces presented in **Nopens *et al.* (2009)** have been modified to link the modified activated sludge model and the anaerobic digestion model (**Batstone *et al.*, 2002**), by considering COD, N and charge balances for all oxidized nitrogen compounds. At the activated sludge side five new variables are defined compared to the ASM1 model used in BSM2: NO_2^-, NO, N_2O, N_2 and an additional autotrophic biomass (X_{BA2}). Further information about the models used can be found in **Corominas *et al.* (2012)** and **Porro *et al*. (2011)**.

Basic control strategy

The plant is simulated in closed loop regime and includes two PI control loops. The first loop controls the dissolved oxygen concentration in AER2 by means of manipulating the aeration flow. The second loop controls the nitrate concentration in the 2nd anoxic tank (ANOX2) by manipulating the internal recycle flow rate (Q_{intr}). Two different waste sludge flow rates (Q_W = 300 $m^3.day^{-1}$ // Q_W = 450 $m^3.day^{-1}$) are imposed in SEC depending on the time of the year in order to sustain the nitrifying biomass in the system during the winter period. Noise and delays are applied to sensors and actuators to give the simulations more realism. External recirculation flow rate (Q_r) and carbon source addition (Q_{carb}) remain constant. Additional details about the operational strategy can be found in **Flores-Alsina *et al.* (2011)**.

Simulated scenarios

Three different scenarios are simulated assuming variations in the TSS removal efficiency of PRIM. In the primary clarifier model used in the BSM2 model, TSS are concentrated into the sludge stream based on an empirical expression taking into account the hydraulic retention time and the ratio of particulate to total COD. The model parameters are defined to produce a TSS concentration in the sludge stream equal to 3% for the average dry weather influent wastewater and a TSS removal efficiency of 50%. In the alternative scenarios the TSS removal efficiency is set to 33% and 66%, respectively. Further information about the primary clarifier model can be found in **Otterpohl and Freund (1992)** and **Otterpohl *et al.* (1994)**.

Evaluation of the effluent quality (EQI) and the operational cost (OCI) indices

The overall pollution removal efficiency is obtained using the effluent quality index (EQI) from the standard BSM2 (**Nopens *et al.*, 2010**). EQI is an aggregated index of all the pollution loads TSS, COD, BOD_5, total Kjeldahl nitrogen (TKN) and NO_X leaving the plant. The economic objectives are evaluated using the operational cost index (OCI) (**Nopens *et al.*, 2010**). It consists of all the major operating costs in the plant: aeration energy (AE), pumping energy (PE), mixing energy (ME), sludge production (SP), external carbon addition (EC), methane production (MP) and the net heating energy (HE^{net}) needed to heat the sludge in the AD. EQI and OCI are based on one-year dynamic influent data generated following the principles stated in **Gernaey *et al.* (2011)**.

Evaluation of greenhouse gas emissions

The GHG emissions included are indicated in **Figure 1**. The comprehensive method proposed by **Flores-Alsina *et al.* (2011)** is used to calculate GHG emissions in the WWTP**.** The emissions considered are:

Direct secondary treatment emissions: The emission from the activated sludge section 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.

Sludge processing: The GHG emissions during sludge treatment are mainly generated in the anaerobic digester. In this case it is assumed that the biogas is fed directly into a gas-fired combustion turbine converting the CH_4 into CO_2 and generating electricity and heat (in turn used to heat the anaerobic digester). The CO_2 generated during anaerobic digestion and the CO_2 produced in the combustion are released to the atmosphere.

Net power GHG: The difference between energy usage and production. Energy consumption involves aeration, pumping, mixing and heating. Energy production comes from the electricity generated by the turbine. A value of 0.94 kg CO_2 per kWh is assumed for any external energy production (based on a coal plant (**Bridle *et al*., 2008**)).

Chemicals: The GHG emissions from production of carbon source for denitrification are accounted for (from industrial production of methanol data) (**Dong and Steinberg, 1997**).

Sludge disposal and reuse: The disposal of sludge is accounted for with CO_2 emissions from transport and mineralization of organic matter to/at the disposal site.

Following the same principles as for EQI and OCI, GHG emissions are evaluated over one year. Finally, in order to deal with the different nature of the generated GHG emissions (CO_2, CH_4 and N_2O), energy credit ($kWh.day^{-1}$) and methanol usage ($kg.day^{-1}$), all emissions are converted into units of CO_2 equivalents (CO_{2e}). The assumed global warming potential (GWP) for N_2O and CH_4 is 298 kg CO_{2e} per kg N_2O and 25 kg CO_{2e} per kg CH_4, respectively (**IPCC, 2006**).

RESULTS

Tables 1, 2 and **3** show the effluent quality, economical and GHG criteria. High PRIM efficiency (TSS removal = 66%) decreases the quantity of TSS entering the activated sludge (AS) section leading to better effluent quality (although denitrification really worsened because of lack of carbon source). The lower operation cost is due to: i) better energy recovery in the sludge line (see **Figure 2a**) and ii) lower aeration cost, but it increases the overall N_2O emissions due to low C/N ratio as a trade-off (see **Figure 2b**).

Table 1. Average effluent quality variables for the three evaluated scenarios

removal	33%	50%	66%	units
TKN	4.6	3.8	3.5	$g.m^{-3}$
N-tot	13.0	13.4	14.2	$g.m^{-3}$
COD	56.7	49.7	48.4	$g.m^{-3}$
BOD	4.2	3.2	3.1	$g.m^{-3}$
TSS	20.6386	15.3510	14.2855	$g.m^{-3}$
EQI	**6774.8**	**6127.5**	**6099.0**	**$kg.day^{-1}$**

In terms of GHG emissions (**Table 3**), low clarifier efficiency i) increases the biogenic CO_2 emissions from BOD oxidation and biomass decay in the bioreactor, ii) increases off-site CO_2 emissions due to higher energy demand during nitrification, iii) reduces energy recovery from settled organics (**Figure 2a**) and iv) decreases N_2O emissions due to a high C/N ratio (**Figure 2b**).

Table 2. Relative costs for the three evaluated scenarios

removal	33%	50%	66%	units
AE	**5707.2**	**5339.0**	**4941.9**	-
PE	**472.5**	**420.5**	**375.3**	-
EC	6000.0	6000.0	6000.0	-
ME	708.0	708.0	708.0	-
HE	0.0	0.0	0.0	-
MP	-5797.3	-6777.0	-7730.9	-
OCI	**15038.3**	**13791.3**	**12407.1**	-

Figures 2a and **b** show the seasonal variation of CH_4 and N_2O (starting date 1st of July). In winter time CH_4 production is reduced due to the reduced waste flow and consequent accumulation of biomass in the AS instead of sending the sludge to the AD. N_2O emissions are decreased during winter time due to incomplete nitrification.

DISCUSSION

The results reported in this paper reach similar conclusions as the experiments reported in **Schulthess and Gujer (1996),** related to C/N ratios and N_2O emissions. There is also a good match with the studies of the effect of soluble/particulate compounds in the AS and the relation with the overall GWP of the plant (**Gori *et al.*, 2011**). Nevertheless, there are aspects that still need to be addressed. For example, there is evidence that N_2O production increases during winter time (**Kampschreur *et al.*, 2009**). In our case, lower temperatures have the opposite effects (see **Figure 2a**).

The authors are aware of the fact that a TSS removal of 66% in PRIM is hard to achieve in many treatment plants without the addition of chemicals (**Tchobanoglous *et al.*, 2003**). Further research is necessary to consider the role of these chemicals within the operational cost index and the overall GWP in a similar way as is done for carbon source usage, i.e. kg CO_{2e} for each kg of chemical used.

Table 3. GHG emissions for the three different scenarios (per m^3 of treated wastewater)

removal	33%	50%	66%	units
Biomass respiration	202.8	180.0	152.2	g CO_{2e} .m^{-3}
BOD oxidation	245.2	211.6	176.7	g CO_{2e} .m^{-3}
Credit nitrification	-11.1	-11.5	-11.8	g CO_{2e} .m^{-3}
N_2O emissions	490.1	586.6	731.9	g CO_{2e} .m^{-3}
Total secondary treatment	**927.1**	**966.7**	**1049.1**	**g CO_{2e} .m^{-3}**
CO_2 emissions from digestion	67.0	78.5	89.9	g CO_{2e} .m^{-3}
CH_4 production from digestion	128.6	150.3	171.4	g CO_{2e} .m^{-3}
Total sludge processing	**195.6**	**228.8**	**261.3**	**g CO_{2e} .m^{-3}**
Power consumption	313.3	294.2	274.0	g CO_{2e} .m^{-3}
Power generation	-262.5	-306.9	-350.1	g CO_{2e} .m^{-3}
Net energy	**50.7**	**-12.7**	**-76.1**	**g CO_{2e} .m^{-3}**
Chemical use	**99.4**	**99.4**	**99.4**	**g CO_{2e} .m^{-3}**
Sludge for disposal	**189.5**	**193.1**	**193.4**	**g CO_{2e} .m^{-3}**
Total emissions	**1462.3**	**1475.3**	**1527.1**	**g CO_{2e} .m^{-3}**

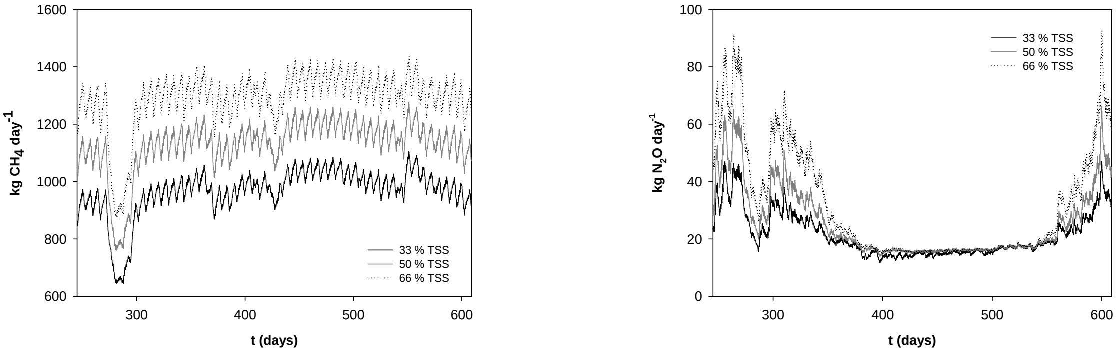

Figure 2. Dynamic profiles of: a) CH_4 in the AD for energy recovery and b) N_2O emissions from AS for the three evaluated scenarios.

Even though the results seem very specific, the presented tool is rather general. The influent characteristics (**Gernaey *et al*., 2011**) and the WWTP design (**Nopens *et al*., 2010**) can be customized for different situations. In case of doing so, the environmental impact of the different pollutants used to quantify the EQI has to be changed. Also, future users will have to update the relative importance of energy, chemicals and sludge treatment and collection costs used to quantify the OCI. Regarding the parameters used to quantify the different GHG emissions, some changes may be necessary. For example, i) the external energy source will have a strong influence when converting kWh.day^{-1} to kg CO_{2e} day^{-1}, ii) the utilization (or not) of biogas for sludge heating and plant electricity (cogeneration), iii) transport distances and iv) the sludge fate (incineration, landfill…) might change from one case to another. Taking these factors into account the presented set of models can be used as a decision support tool for process managers, water authorities and regulators when evaluating the sustainability of different engineering applications as: i) design, ii) process optimization and iii) evaluation of alternatives for plant upgrading/expansion.

The case study show that the presented models are useful to quantify the different GHG emissions resulting from certain control strategies/operational procedures taking into account the different sources of CO_2, CH_4 and N_2O. However, from a climate change point of view, not all these sources have the same importance. For example, biogenic sources of CO_2 such as the generation from the aerobic/anaerobic treatment processes are part of the natural carbon cycle. On the other hand, there are non-biogenic sources such as the off-site CO_2 emissions due to electricity consumption or production of chemicals that should be avoided.

Some of the models used in the case study are still under development. In this paper the N_2O production is based on AOB denitrification with NO_2 as terminal electron acceptor. However, other possible mechanisms, such as the formation of N_2O as a by-product of incomplete oxidation of hydroxylamine (NH_2OH) to NO_2, are omitted. Recent investigations demonstrate that both the denitrification and NH_2OH pathways may be involved in N_2O production. Unfortunately, a unified model that describes both mechanisms independently does not yet exist (**Ni *et al*., 2012**).

Finally, the reader should be aware that the list of emissions applied in this case study is not complete. There are other sources of GHG that potentially contribute to the overall GWP of the plant. Experimental observations have revealed that substantial stripping of methane might take place at the inlet of the WWTP (**Guisasola *et al*., 2009**). Also, no fugitive emissions of methane are considered from the anaerobic digester (**Czepiel *et al*., 1993**). In the ADM-ASM interfaces (**Nopens *et al*., 2009**), the quantity of methane that remains in the liquid phase is stripped, but not quantified. Finally, the N_2O and CH_4 emissions from sludge disposal and reuse are not considered either (**EPA, 2010**).

CONCLUSIONS

The key findings of the presented study can be summarized in the following points:

- A set of dynamic models to quantify GHG emissions in WWTP was presented;
- A simplified case study showed the synergies and trade-offs between effluent quality, operational cost and GHG emissions when the TSS removal efficiency in PRIM was modified;
- Modelling results match to a large extent experiments that can be found in the literature. However, there are still issues that need to be addressed;
- Even though results are shown for the BSM2, the presented tools are rather generic and can easily be adapted to specific situations;
- Quantification of GHG emissions is an expanding research field and is evolving rapidly. Some models are still not available, or under development. However, the presented set of models provides a fair representation of reality and demonstrates the usefulness of a framework to quantify plant-wide emissions for various control strategies.

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