Science of the Total Environment 466–467 (2014) 616–624

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Balancing effluent quality, economic cost and greenhouse gas emissions during the evaluation of (plant-wide) control/operational strategies in WWTPs

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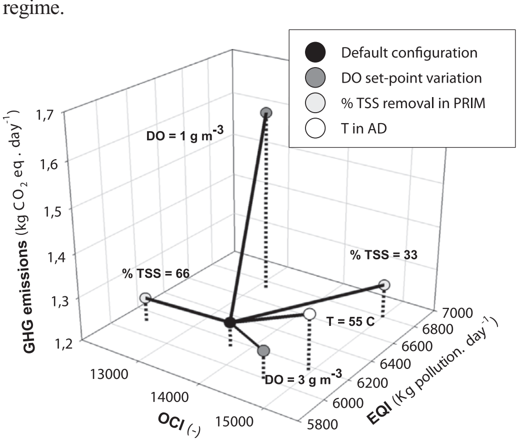
HIGHLIGHTS

- A 3-D graphical representation shows the interactions among effluent quality, operational cost and GHG emissions during the evaluation of operational/control strategies in WWTP.
- The study points out the importance of taking into account the existing interactions among the water and sludge line.
- The potentially undesirable effects of local energy optimization (aeration/biogas) are highlighted when calculating the total plant's overall global warming potential.

GRAPHICAL ABSTRACT

The 3-D representation of effluent quality (EQI), operational cost (OCI) and greenhouse gas emissions (GHG) during the evaluation of several (plant-wide) control/operational strategies: (1) modification of the DO set point, (2) modification of the primary clarifier TSS removal efficiency and (3) modification of the anaerobic digester temperature regime.



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http://dx.doi.org/10.1016/j.scitotenv.2013.07.046

A R T I C L E   I N F O

Article history:
Received 2 April 2013
Received in revised form 2 July 2013
Accepted 13 July 2013
Available online xxxx

Editor: Simon Pollard

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

A B S T R A C T

The objective of this paper was to show the potential additional insight that result from adding greenhouse gas (GHG) emissions to plant performance evaluation criteria, such as effluent quality (EQI) and operational cost (OCI) indices, when evaluating (plant-wide) control/operational strategies in wastewater treatment plants (WWTPs). The proposed GHG evaluation is based on a set of comprehensive dynamic models that estimate the most significant potential on-site and off-site sources of CO_2, CH_4 and N_2O. The study calculates and discusses the changes in EQI, OCI and the emission of GHGs as a consequence of varying the following four process variables: (i) the set point of aeration control in the activated sludge section; (ii) the removal efficiency of total suspended solids (TSS) in the primary clarifier; (iii) the temperature in the anaerobic digester; and (iv) the control of the flow of anaerobic digester supernatants coming from sludge treatment. Based upon the assumptions built into the model structures, simulation results highlight the potential undesirable effects of increased GHG production when carrying out local energy optimization of the aeration system in the activated sludge section and energy recovery from the AD. Although off-site CO_2 emissions may decrease, the effect is counterbalanced by increased N_2O emissions, especially since N_2O has a 300-fold stronger greenhouse effect than CO_2. The reported results emphasize the importance and usefulness of using multiple evaluation criteria to compare and evaluate (plant-wide) control strategies in a WWTP for more informed operational decision making.

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1. Introduction

The main focus in assessing the operation of wastewater treatment plants has historically been the effluent water quality under constraints of technical feasibility and cost. This certainly still holds, but the discussions on sustainability in general and the issue of climate change due to greenhouse gas (GHG) emissions in particular (Foley et al., 2011; Law et al., 2012; Rodriguez-Garcia et al., 2012) have widened the scope for the utilities. An increasing interest in GHG emissions calls for novel approaches to evaluate the performance of control and operational strategies in order to include additional performance indicators related to GHG emissions.

Aside from evaluating control and operational strategies (Nopens et al., 2010) before full-scale implementation (Ayesa et al., 2006), dynamic activated sludge models (ASM) (Henze et al., 2000) have been widely used for multiple purposes in wastewater engineering such as benchmarking (Gernaey et al., 2013), diagnosis (Olsson, 2012; Rodriguez-Roda et al., 2002), design (Rieger et al., 2012; Flores et al., 2007), teaching (Hug et al., 2009) and optimization (Rivas et al., 2008). Based on new knowledge on the chemical and biochemical mechanisms of GHG production, recent efforts have been made to capture the production and emissions of CO_2, CH_4 and N_2O and integrate these processes in the traditional ASM models (Batstone et al., 2002; Hiatt and Grady, 2008; Ni et al., 2013; Mampaey et al., 2013; Guo and Vanrolleghem, 2013).

Nevertheless, there are few studies discussing the additional benefit of adding a new dimension related to GHG production and emission to the traditional effluent quality and operational cost indices within the performance evaluation procedures (Flores-Alsina et al., 2011; Corominas et al., 2012; Guo et al., 2012). In this paper, an extended version of the International Water Association (IWA) Benchmark Simulation Model No. 2 (BSM2), i.e., BSM2G, is used for all simulations to demonstrate the benefit of adding this additional GHG emissions dimension.

A novelty of this paper includes the evaluation of plant-wide control/operational strategies through an integrated GHG modeling approach, representing the major pathways known to contribute significantly the plant-wide carbon footprint. These strategies involve changes related to the following process variables: (i) the dissolved oxygen (DO) set point of the aeration system in the activated sludge section; (ii) the removal efficiency of the total suspended solids (TSS) in the primary clarifier; (iii) the temperature in the anaerobic digester (AD); and (iv) the control of the flow of anaerobic digester supernatants from sludge treatment. Further, the authors in this paper consider the main interactions between the water and the sludge line. Finally, changes in effluent quality index (EQI), operational cost index (OCI) and CO_2, CH_4 and N_2O emissions are analyzed by means of a 3-D representation and thoroughly discussed. As a side effect, synergies and trade-offs between local energy optimization and the overall GHG production is studied in detail.

2. Methods

2.1. Wastewater treatment plants under study

The WWTP under study (BSM2G) has the same layout as the IWA BSM2 platform proposed by Nopens et al. (2010). The plant is treating an influent flow rate of 20,648 $m^3 \cdot day^{-1}$ and a total COD and N load of 12,240 and 1140 $kg \cdot day^{-1}$, respectively. Influent characteristics are generated following the principles stated in Gernaey et al. (2011). The activated sludge (AS) unit is a modified Ludzack-Ettinger configuration consisting of 5 tanks in series. Tanks 1 (ANOX1) and 2 (ANOX2) are anoxic (total volume = 3000 m^3), while tanks 3 (AER1), 4 (AER2) and 5 (AER3) are aerobic (total volume = 9000 m^3). AER3 and ANOX1 are linked by means of an internal recycle with the purpose of nitrate recycle for pre-denitrification. The BSM2G plant further contains a primary (PRIM) (900 m^3) and a secondary (SEC) clarifier (6000 m^3), a sludge thickener (THK), an anaerobic digester (AD) (3400 m^3), a storage tank (ST) (160 m^3) and a dewatering unit (DW). Additional information about the plant design and operational conditions can be found in Flores-Alsina et al. (2011).

The biological process model used in the study is described in detail in Guo and Vanrolleghem (2013). From the original set of models of BSM2, the Activated Sludge Model No. 1 (ASM1) (Henze et al., 2000) has been expanded with the principles proposed by Hiatt and Grady (2008) and Mampaey et al. (2013). The Hiatt and Grady model incorporates two nitrifying populations: ammonia oxidizing bacteria (AOB) and nitrite oxidizing bacteria (NOB) using free ammonia (NH_3) and free nitrous acid (FNA) as nitrogen substrate, respectively. The model also considers sequential reduction of nitrate (NO_3^-) to nitrogen gas (N_2) via nitrite (NO_2^-), nitric oxide (NO) and nitrous oxide (N_2O) using individual reaction-specific parameters. Additionally, the ideas summarized in Mampaey et al. (2013) are used to consider NO and N_2O formation from the nitrification pathway assuming ammonia (NH_3) as the electron donor. To account for seasonal variability, liquid–gas saturation constants, kinetic parameters, transfer coefficients and equilibrium reactions are temperature dependent. Stripping equations for the gases were implemented as in Foley et al. (2011). 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. Further information about the GHG models and parameter values can be found in Corominas et al. (2012) and Guo et al. (2012).

Nomenclature

AD	anaerobic digester
ADM	anaerobic digestion model
AE	aeration energy ($kWh \cdot day^{-1}$)
AER	aerobic section
AOB	ammonium oxidizing bacteria
ANOX	anoxic section
ASM	activated sludge model
BOD	biochemical oxygen demand ($g \cdot m^{-3}$)
BSM2	Benchmark Simulation Model No 2
CH_4	methane (kg $CH_4 \cdot day^{-1}$)
CO_2	carbon dioxide (kg $CO_2 \cdot day^{-1}$)
CO_2e	equivalent carbon dioxide (kg $CO_{2e} \cdot day^{-1}$)
COD	chemical oxygen demand ($g \cdot m^{-3}$)
DO	dissolved oxygen concentration ($g \cdot m^{-3}$)
DW	dewatering unit
EC	consumption of external carbon source (kg $COD \cdot day^{-1}$)
EQI	effluent quality index (kg $pollution \cdot day^{-1}$)
GHG	greenhouse gas
GWP	global warming potential
HE	heating energy ($kWh \cdot day^{-1}$)
k_La	volumetric oxygen transfer coefficient (day^{-1})
ME	mixing energy ($kWh \cdot day^{-1}$)
MP	methane production (kg $CH_4 \cdot day^{-1}$)
N	nitrogen
NH_4^+	ammonium nitrogen (g $N \cdot m^{-3}$)
NO	nitric oxide nitrogen (g $N \cdot m^{-3}$)
N_2O	nitrous oxide nitrogen (kg $N \cdot day^{-1}$)
NOB	nitrite oxidizing bacteria
NO_2^-	nitrite nitrogen (g $N \cdot m^{-3}$)
NO_3^-	nitrate nitrogen (g $N \cdot m^{-3}$)
NO_x	oxidized forms of nitrogen (g $N \cdot m^{-3}$)
OCI	operational cost index (cost $unit \cdot year^{-1}$)
PE	pumping energy ($kWh \cdot day^{-1}$)
PRIM	primary clarifier
PI	proportional integral controller
Q_{carb}	external carbon source flow rate ($m^3 \cdot day^{-1}$)
Q_e	effluent flow rate ($m^3 \cdot day^{-1}$)
Q_{intr}	internal recycle flow rate ($m^3 \cdot day^{-1}$)
Q_r	external recirculation flow rate ($m^3 \cdot day^{-1}$)
Q_w	waste sludge flow rate ($m^3 \cdot day^{-1}$)
SEC	secondary clarifier
SP	sludge production (kg $TSS \cdot day^{-1}$)
SRT	sludge retention time (day)
ST	storage tank
THK	thickener
TKN	total Kjeldahl nitrogen ($g \cdot m^{-3}$)
TN	total nitrogen ($g \cdot m^{-3}$)
TSS	total suspended solids ($g \cdot m^{-3}$)
WWTP	wastewater treatment plant

2.2. Control strategy and simulated scenarios

The plant is simulated in a closed loop regime, which includes two PI control loops. The first loop controls the dissolved oxygen concentration in AER2 by manipulating the air supply rate, here implemented as the oxygen transfer coefficient K_La4 (set point = 2 g O_2 $g \cdot m^{-3}$). K_La3 is set equal to K_La4 and K_La5 is set to half its value. The second loop controls the nitrate concentration in ANOX2 by manipulating the internal recycle flow rate (Q_{intr}). Two different waste sludge flow rates (Q_{w_winter} = 300 $m^3 \cdot day^{-1}$ // Q_{w_summer} = 450 $m^3 \cdot day^{-1}$) 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 sensor and actuator models to give the simulations more realism. The external recirculation flow rate (Q_r) and carbon source addition (Q_{carb}) remain constant throughout the simulations. Additional details about the default operational strategy can be found in Flores-Alsina et al. (2011). The selection of the different scenarios is intended to demonstrate the relative effects of logical control strategies that may be implemented by operators to increase energy efficiency and/or improve overall plant performance. The following four selected scenarios are simulated in the presented case study:

- Impact of DO control (commonly used to reduce aeration costs) by varying the set point value between 1 and 3 $g \cdot m^{-3}$ (default value 2 $g \cdot m^{-3}$).
- Impact of primary clarifier efficiency by varying the TSS removal efficiency in PRIM from 33% to 66% (default value 50%). Although in reality this does not happen without chemical addition, the effect of improving TSS removal, such as through chemical addition, is the change of interest.
- Impact of the anaerobic digester operating mode by changing the temperature in the anaerobic digester from mesophilic (35 °C) to thermophilic (55 °C) (default value 35 °C).
- Impact of anaerobic digester supernatants by controlling the return flow rate originating from the DW unit. This timer-based control strategy stores the dewatering liquor during daytime (when the plant is high loaded) and returns it at night (when the plant is low loaded). Note that the default BSM2 strategy does not use this control approach and liquors are simply returned as they are generated.

2.3. Evaluation criteria

2.3.1. Effluent quality (EQI) and 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 weighted index of all pollution loads: TSS, COD, BOD_5, total Kjeldahl nitrogen (TKN) and the oxidized forms of nitrogen (NO_X), leaving the plant. The economic objectives are evaluated using the operational cost index (OCI) (Nopens et al., 2010). It consists of the sum of all 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}). EQI and OCI are based on simulation results with the 609 days of dynamic influent data generated following the principles outlined in Gernaey et al. (2011), although only the last 364 days are used for the evaluation itself.

2.3.2. Greenhouse gas (GHG) emissions

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 emissions from the activated sludge section include the CO_2 generated from biomass respiration and BOD oxidation, the N_2O generated from nitrogen removal and the CO_2 credit from nitrification. Although in theory possible from anaerobic digester supernatants return and from the influent, CH_4 stripping/emissions in the secondary treatment were not considered, as they are not yet predicted by the plant-wide models.
- 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 influent). The CO_2 generated during anaerobic digestion and the CO_2 produced in the combustion process are assumed to be 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 $CO_2 \cdot (kWh)^{-1}$ is assumed for any external energy production required (based on the efficiency of a coal-burning power 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 by CO_2 emissions from transport and mineralization of organic matter at the disposal site considering three different fates. Compost (45 %) and agriculture (38%) are the main fates, while a small fraction is sent to forestry (17 %). When it comes to transport, forestry and agriculture imply further distance (≈150 km) than compost (≈20 km).

GHG emissions are also evaluated over a one-year period following the same principles. Finally, in order to deal with the different nature of the generated GHG emissions (CO_2, CH_4 and N_2O) they are converted into units of CO_2 equivalents (CO_2e). The assumed global warming potentials (GWP) for N_2O and CH_4 are 298 kg CO_2e per kg N_2O and 25 kg CO_2e per kg CH_4, respectively (IPCC, 2007).

It is important to highlight that this methodology accounts for the main sources of GHG emissions. However, the selected types of emissions and how they are included in the evaluation procedures can be user-defined based on various objectives and boundaries of interest. For example, it is possible to break down the plant's global warming potential into biogenic/non-biogenic emissions or within (on-site) and outside (off-site) the fence emissions.

3. Results

EQI, OCI and GHG values for the different simulated scenarios are shown in Fig. 1. As mentioned previously, the selection of the different scenarios is intended to demonstrate the relative effects of logical control strategies that may be implemented by operators to optimize plant performance. However, the main underlying reason for the scenario selection is the desire of showing the benefit of including the additional dimension dealing with GHG emissions when implementing changes across the whole plant. This is highlighted by moving from the 2-D to the 3-D representation and showing the results for a variety of situations. Hence, it is possible to see how the overall picture changes when (1) EQI and OCI are considered only or (2) when adding the total quantity of CO_2, N_2O and CH_4 emissions (quantified in kg $CO_2e.\ m^{-3}$ of treated wastewater). From the generated results one can see that (1) the dissolved oxygen set point in the activated sludge section has a paramount importance on the plant's total GHG emissions (*z*-axis) next to the well-known impacts on effluent quality and operating costs; (2) better TSS removal efficiency in PRIM mainly improves effluent quality and operational cost (*x*- and *y*-axes), but the total GHG emissions remain almost equal; (3) thermophilic conditions in the anaerobic digester reveal that a higher operating temperature appears to be a more expensive way to operate the plant (with higher operational cost, *y*-axis) without having substantial benefits in terms of increased gas production (Fig. 4); and (4) control of the anaerobic digester supernatants return flow rate slightly improves effluent quality, increases cost but does not have an effect on the GHG emissions unless

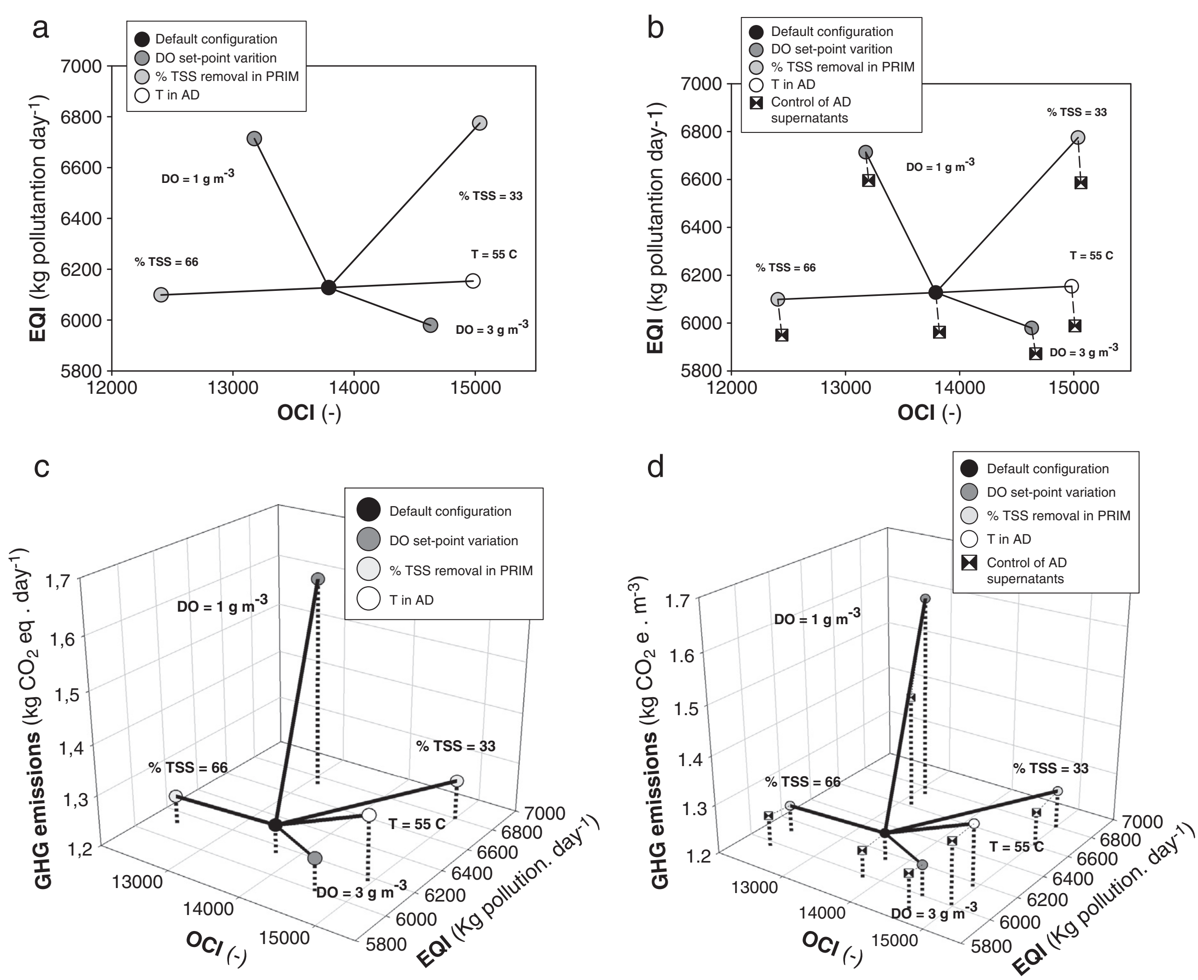

Fig. 1. Effluent quality (a, b, c, d), operational cost (a, b, c, d) and greenhouse gas emissions (c, d) for the different control strategies with (b, d) and without (a, c) controlling the anaerobic digester supernatant.

DO is very low (see dotted lines in Fig. 1, right). Figs. 2–4, show the dynamic variation of selected process variables and their seasonal variation (simulation start date: 1st of July, day = 245, total time: 364 days). Further details and discussion of these results are provided in the following sub-sections.

3.1. Effect of dissolved oxygen concentration

Low DO set points lead to a reduction of the off-site CO_2 production due to lower energy consumption and subsequently lower operational cost (detailed results not shown), but the overall GHG emissions are increased compared to the default case. The reason for this GHG increase is the increased formation of N_2O and its approximately 300-fold stronger greenhouse effect compared to CO_2. In this case, the N_2O increase is mainly caused by accumulation of NO_2^- (see Fig. 2, right) due to incomplete nitrification (see the increase of the EQI values in Fig. 1 and the dynamics of NH_4^+ in Fig. 2, left). High DO set points increase aeration energy and operational costs but improve effluent quality (see *x*- and *y*-axes in Fig. 1 and dynamic profiles in Fig. 2). Despite higher off-site emissions of CO_2, the overall GHG emissions are still lower due to a reduced N_2O contribution. In all cases (Figs. 2–4), the sudden drop around day 290 is caused by the holidays simulated in summer (for further details, see Gernaey et al., 2011).

3.2. Effect of primary clarifier efficiency

High PRIM efficiency (TSS removal = 66%) decreases the quantity of TSS entering the activated sludge section and improves the overall nitrification efficiency leading to better effluent quality (even though denitrification is significantly worsened because of a lack of readily biodegradable organic material). There is a reduction in the operational cost mainly due to (i) the lower aeration energy in the activated sludge section and (ii) the increased biogas production, which leads to higher energy recovery in the sludge line (see Fig. 3, right). However, the lower organic load entering the biological reactor increases the overall N_2O emissions due to the low C/N ratio of the primary clarifier effluent (see Fig. 3, left), especially in warm temperatures (days 245 to 350 and 550 to 609). Conversely, a low PRIM efficiency (TSS removal = 33%) decreases the effluent quality due to reactor overloading. Operational costs are higher due to (i) increased energy demand in the aerobic section and (ii) low energy recovery from the sludge line. In terms of GHG emissions, lower TSS removal in PRIM causes (i) an increase of the CO_2 emissions from BOD oxidation and biomass decay in the bioreactor and (ii) higher off-site CO_2 emissions due to increased energy demand in the aerobic section and low-energy recovery in the AD. All in all, the overall variations of the total GHG emissions seem to be very small when changing PRIM efficiency (*z*-axis in Fig. 1). However, the specific GHG compounds emitted and their origin change substantially in the different simulated scenarios (see the discussion section).

3.3. Effect of digester performance

Fig. 4 shows the results of changing the digester's operating temperature from 35 °C (mesophilic conditions) to 55 °C (thermophilic conditions). In this system, no substantial benefits can be observed in either biogas production or off-site CO_2 emissions. However, thermophilic conditions substantially increase the operational cost (Fig. 1) due to higher energy requirements for heating (Fig. 4, left) without significantly improving the digester performance (Fig. 4, right). Subsequently, this also leads to higher CO_2 emissions from off-site power generation. The effect on effluent quality variables is negligible (see discussion section).

3.4. Effect of controlling the return flows of anaerobic digester supernatants

In Fig. 1, the effect of controlling the anaerobic digester supernatants return flows is shown. In all cases, there is a slight improvement in the effluent quality (all evaluated scenarios have lower values of the EQI, *x*-axis) when control of the anaerobic digester supernatants returns is activated. This reduction is attributed to the storage tank's capability to reduce the effect of ammonium peaks originating from the sludge treatment line when the plant is already high loaded. Fig. 5 shows the smoothing effect on the effluent ammonium nitrogen of controlling the anaerobic digester supernatants return flows. On the other hand, the slight increase in the OCI (*y*-axis) of Fig. 1 is due to the extra pumping. Finally, with regard to GHG generation, there is no substantial benefit unless the DO concentration is very low. As mentioned before, low DO levels combined with high ammonium loads substantially increase the total N_2O emissions. The simulation results show that N_2O decrease can be achieved by dampening the ammonium peaks.

4. Discussion

The results reported in this case study pave the way to several discussions. Indeed, the additional dimension provided by the quantification of the N_2O, CH_4 and CO_2 generation from the WWTP changes the overall picture of the evaluation procedure giving a better idea about the "sustainability" of the different alternatives.

4.1. Importance of plant-wide control

The study presents an important result to the wastewater community showing the potential impacts of energy optimization, particularly in the aeration/anaerobic digester system and the importance of plant-wide evaluation. For example, Fig. 1 shows the clear advantages of increasing the % TSS removal in the PRIM. Firstly, the load to the activated

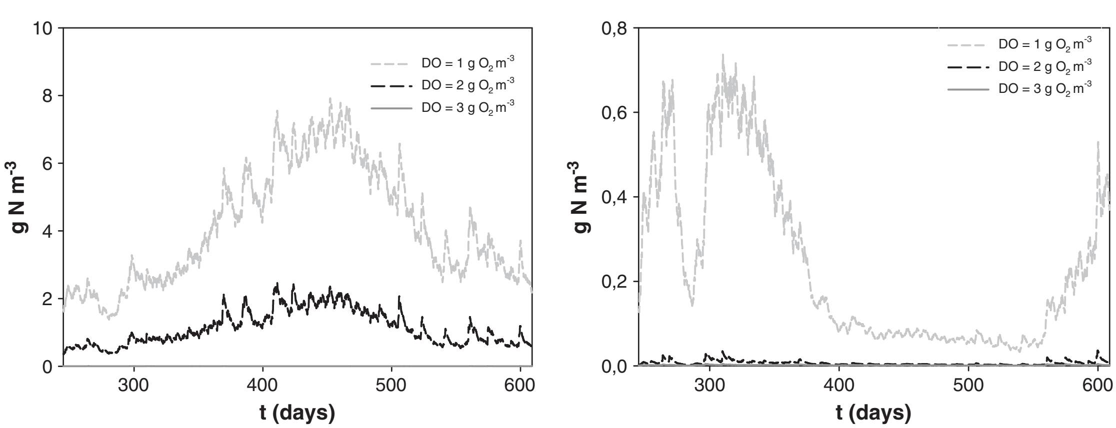

Fig. 2. Effect of dissolved oxygen on nitrification: NH_4^+ (left) and NO_2^- (right) in the effluent.

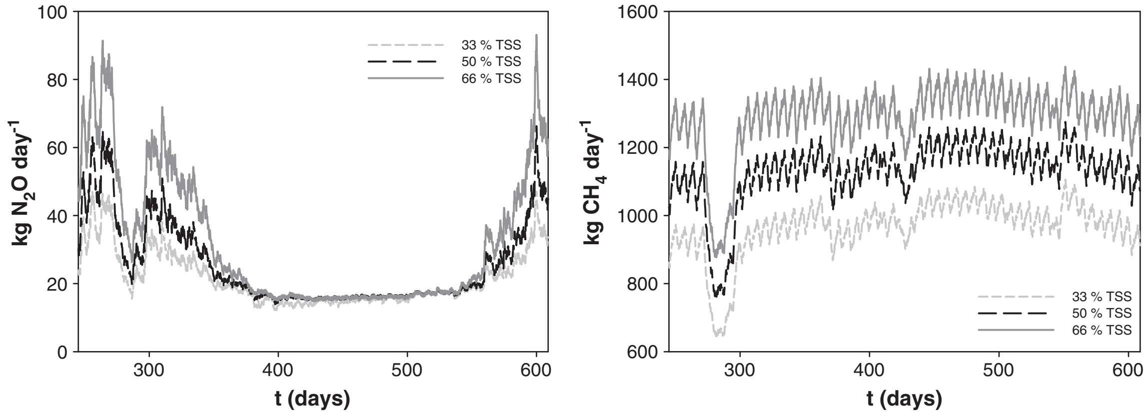

Fig. 3. Effect of TSS removal efficiency in PRIM: N_2O emissions from the activated sludge (left) and CH_4 from the anaerobic digester (right).

sludge section is substantially reduced (and thus the off-site CO_2 emissions due to aeration). Secondly, there is an increase of energy recovery from the anaerobic digestion (higher CO_2 credit). However, the total quantity of GHG emissions does not change since there is a substantial increase of N_2O emissions due to the inadequate C/N ratios that result (poor denitrification). Finally, this analysis provides insights with regard to decision making and evaluating operational options. Indeed, based on the results, operating a plant at low DO concentrations cannot be recommended due to the decrease in effluent quality despite the substantial savings in OCI (see Fig. 1a, b). The situation becomes even worse when GHG emissions are included in the analysis (Fig. 1c, d) and the substantial contribution of N_2O in the total plant's global warming potential would rank that alternative even lower. This demonstrates the usefulness of a third GHG dimension for deciding on the optimum DO control strategy to meet a specific plant's objectives.

4.2. The case study

As the integrated GHG modeling framework used in this paper incorporates AOB denitrification and heterotrophic denitrification N_2O pathways, it is promising to see the results reported in this paper lead to similar observations as the experiments reported in von Schulthess and Gujer (1996) and Kampschreur et al. (2009), related to DO, C/N ratios and N_2O emissions, which helps to validate the models' assumptions and structures and gain confidence in the relative effects observed. There is also good agreement with the studies of the effects of soluble/particulate compounds in activated sludge processes and their relation with the overall GWP of the plant (Gori et al., 2011). However, there are also aspects that warrant further attention. For example, there is suggested evidence that N_2O production increases during winter time (Kampschreur et al., 2009), although lower winter emissions have been reported as well (Daelman et al., 2013). With the ASM1G model used, lower temperatures lead to lower N_2O emissions, as explained in detail by Guo and Vanrolleghem (2013). Further investigations are still being conducted in order to better understand and describe the potential seasonal variability of GHG emissions.

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 such chemicals on the OCI, 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. As mentioned previously, only the TSS removal effect of the chemical is studied in this paper.

Finally, it should be mentioned that traditionally thermophilic conditions should substantially increase biogas production (Tchobanoglous et al., 2003). The limited improvement in digester performance shown in this study can be explained by the following points: (i) the used ASM/ADM interfaces (Nopens et al., 2009) where the disintegration process (limiting factor in many digestion processes) is instantaneous; (ii) the low biodegradable fraction coming with the influent (Gernaey et al., 2011), consequently bringing limited amounts of organic material to the anaerobic digester (although kinetics are faster at thermophilic conditions, there is no more material to be converted); and (iii) the large digester volume, i.e., the digester was originally designed with a sufficiently long hydraulic retention time to convert all potentially digestible organics into methane under mesophilic conditions. If additional external organic waste would be available to make use of the extra digestion capacity in thermophilic conditions, results and conclusions would likely be different.

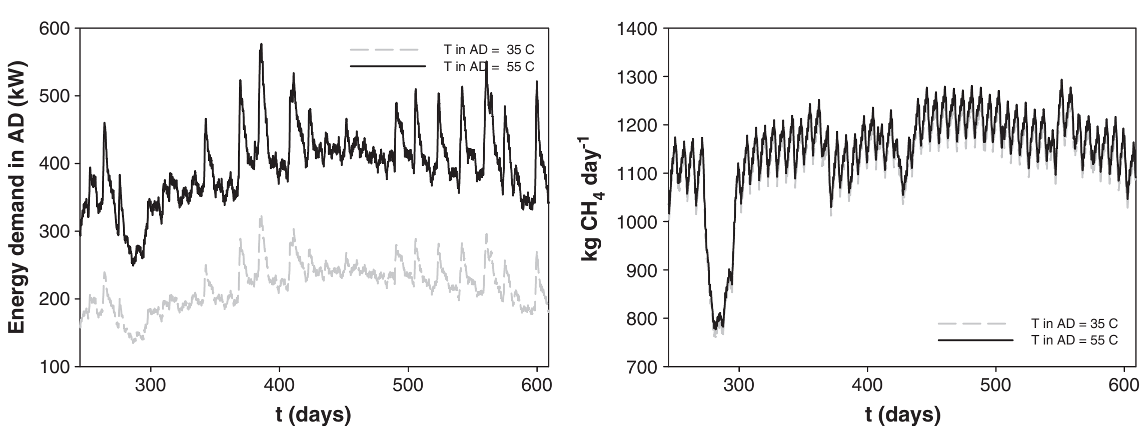

Fig. 4. Effect of modified T regime on the anaerobic digester's performance: energy demand (left) and CH_4 (right) in anaerobic digester.

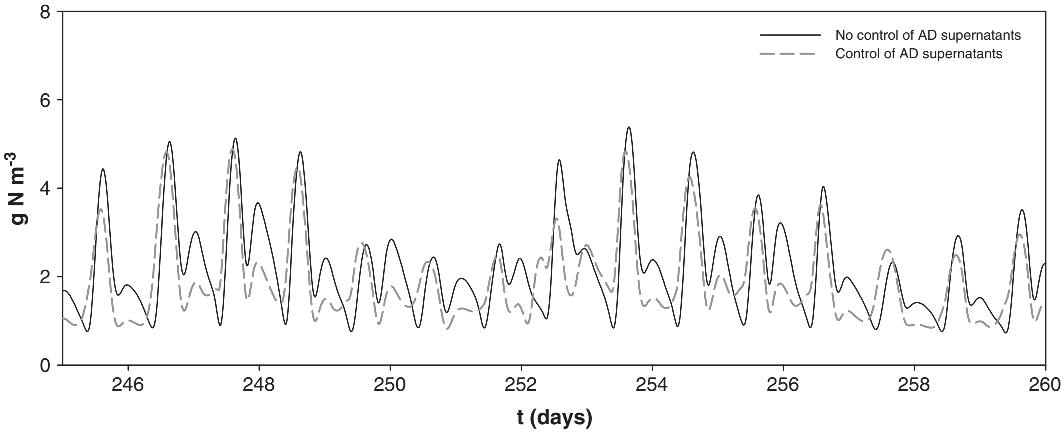

Fig. 5. Effect on the effluent ammonium of controlling the anaerobic digester supernatants (15 day snapshot of 364 days simulation).

4.3. Accounting (framing) for the plant's global warming potential

The case study shows that wastewater treatment system models are useful to quantify the different GHG emissions when evaluating different control strategies or operational procedures by 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 CO_2 emissions from the aerobic/anaerobic treatment of organics contained in the wastewater, are part of the natural carbon cycle, as long as they do not originate from fossil fuel based household products, such as detergents. 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. The methodology presented herein allows making this distinction when computing the plant's overall carbon footprint. A clear example can be found in scenario 2 (% TSS removal efficiency), where the total emission of GHG is almost the same, but their type and origin are quite different. For instance, the percentage of biogenic/ non-biogenic CO_2 varies when the TSS removal efficiency is either decreased or increased: 30/70 and 20/80, respectively.

A similar type of differentiation can be made regarding on-site and off-site emissions. Thus, for the default case study the ratio between off-site and on-site emissions is 0.28. It is important to highlight that this ratio may change for example when the DO set point is decreased or increased. When the DO is decreased and the plant's total energy consumption is decreased (and consequently off-site emissions), the ratio is reduced to 0.18. On the other hand, when the DO set point is increased and there is a high energy demand to maintain 3 g O_2 m^{-3} in the biological reactor, the ratio increases to 0.33 due to higher off-site emission.

4.4. Energy-mix-related consideration issues

It must be noted that the value of 0.94 kg $CO_2e\cdot(kWh)^{-1}$ used for external energy production is an accurate value for a coal-burning power plant, but the electricity mix of any given country can be quite different than sole coal burning (being one of the dirtiest technologies when it comes to CO_2 emissions). In order to evaluate how this value may affect the results of benchmarking studies, the variation in the GWP was also evaluated assuming the average European (0.462 kg $CO_2e\cdot(kWh)^{-1}$) and US (0.731 kg $CO_2e\cdot(kWh)^{-1}$) energy mix value. The effect of DO set point variation is used as an example. Calculations reveal (for this particular case study) that cleaner energy mixes may change the net power GHG ($CO_2e\cdot m^{-3}$) by up to 50%. Nevertheless, the overall effect on the carbon footprint as accounted for in this study will still be very small (<5% in all cases). Note that this percentage may change depending on the framing (biogenic/ non biogenic and on-site/off-site emissions).

4.5. General application of the method

The shown numeric results are case study specific, but the presented tools are generic. The influent characteristics (Gernaey et al., 2011) can be scaled to different situations (Flores-Alsina et al., in press). The same applies for the WWTP design (Nopens et al., 2010), which can be modified to describe full-scale process dynamics (Arnell et al., in press). In a recent study, the same ASM model structure has been tested calibrated/ validated with a SBR plant treating anaerobic digester supernatants (Lindblom et al., in press). Naturally, some of the parameters had to be re-adjusted to better represent the new system, but the match between experiments and simulations was fairly close. It should be stressed that the modification of the model could give an under/overestimation of the total emissions, but the general conclusions would remain almost the same. The reader should be reminded that although the strong weight of N_2O in the GWP of the simulated plant, it is just one of an extensive list of emissions.

The same applies for CH_4 behaviour (Blumensaat and Keller, 2005). In case of doing so, the environmental impact of the different pollutants used to quantify the EQI has to be changed. Moreover, future users will have to update the relative importance of energy, chemicals and sludge treatment and collection costs used to quantify the OCI in accordance to their own (local) requirements.

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 $kWh\cdot day^{-1}$ to kg $CO_2e\cdot day^{-1}$, (ii) the utilization (or not) of biogas for sludge heating and plant electricity (cogeneration), (iii) the transport distances, and (iv) the sludge fate (incineration, landfill etc.) 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 control and process engineers, water authorities and regulators when evaluating the "sustainability" of different engineering applications for (i) design, (ii) process optimization and (iii) evaluation of alternatives for plant upgrading/expansion.

4.6. Limitations

It is important to highlight that the N_2O models used in the study are still under development and are in the process of being validated with full-scale data. Results thus far have been promising (Lindblom et al., in press). In this paper, the N_2O production by AOB is based on denitrification with NH_4^+ as electron donor. 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 not considered. Recent investigations demonstrate that both the autotrophic denitrification and the NH_2OH oxidation are involved in N_2O production, although the latter to a minor degree (Wunderlin et al., 2013). Nevertheless, a unified model that describes both mechanisms independently does not yet exist (Ni et al., 2013). Therefore, the results reflect the assumptions built into the N_2O model structure of Mampaey et al., 2013.

Finally, the reader should be aware that the list of emissions on which this study is based is not complete. There are other sources of GHG that potentially contribute to the overall emissions of the plant. N_2O can be observed in the plant effluent (either because not all N_2O is stripped out in bioreactor or because the effluent NH_4^+ can be converted into N_2O after discharging into the river). 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 or the gas turbine (Daelman et al., 2012). In the ADM–ASM interface (Nopens et al., 2009), the quantity of methane that remains in the liquid phase is stripped, but not quantified in the model. Finally, while CO_2 is included, the potential N_2O and CH_4 emissions from sludge disposal and reuse are not considered either although they might be up to 40% of the total emissions (EPA, 2010; Brown et al., 2010).

5. Conclusions

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

- The inclusion of GHG emissions provides an additional criterion when evaluating control/operational strategies in a WWTP, offering a better idea about the overall "sustainability" of plant control/operational strategies.
- Simulation results show the risk of energy-related (aeration energy in AS/energy recovery from AD) optimization procedures, and the opposite effect that N_2O and its 300-fold stronger GHG effect (compared to CO_2) might have on the overall GWP of the WWTP.
- The importance of considering the water and sludge lines together and their impact on the total quantity of GHG emissions are shown when the temperature regime is modified and the anaerobic digester supernatants return flows controlled.
- While these observations are WWTP specific, the use of the developed tools is demonstrated and can be applied to other systems.

Acknowledgements

The authors acknowledge the financial support obtained through the Swedish Research Council Formas (211-2010-141), the Swedish Water & Wastewater Association (10-106, 11-106), the J. Gust. Richert Memorial Fund (PIAH/11:58), the TECC project of the Québec Ministry of Economic Development, Innovation and Exports (MDEIE) and FWO-Flanders (G.A051.10). Xavier Flores-Alsina gratefully acknowledges the financial support provided by the People Program (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013 under REA agreement 329349 (PROTEUS). Lluís Corominas received the "Juan de la Cierva" scholarship from the Science Ministry of Spain (jci-2009-05604), and the career integration grant (PCIG9-GA-2011-293535) from EU. Laura Snip has received funding from the People Program (Marie Curie Actions) of the European Union's Seventh Framework Programme FP7/2007-2013, under REA agreement 289193 (SANITAS). Peter Vanrolleghem holds the Canada Research Chair in Water Quality Modelling.

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