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Chapter 9

Benchmarking strategies to control GHG production and emissions

Xavier Flores-Alsina[1], Magnus Arnell[2,3], Lluís Corominas[4], Chris Sweetapple[5], Guangtao Fu[5], David Butler[5], Peter A. Vanrolleghem[6], Krist V. Gernaey[1] and Ulf Jeppsson[3]

[1]Process and Systems Engineering (PROSYS) Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Building 228 A, Kgs. Lyngby 2800, Denmark
[2]Unit of Urban Water Management, RISE Research Institutes of Sweden, Gjuterigatan 1D, Linköping SE-58273, Sweden
[3]Division of Industrial Electrical Engineering and Automation (IEA), Department of Biomedical Engineering, Lund University, PO Box 118, Lund SE-22100, Sweden
[4]ICRA, Catalan Institute for Water Research, Scientific and Technological Park, H_2O Building, Emili Grahit 101, Girona 17003, Spain
[5]Centre for Water Systems, College of Engineering, Mathematics and Physical Sciences, University of Exeter, North Park Road, Exeter, Devon EX4 4QF, UK
[6]modelEAU, Département de génie civil et de génie des eaux, Université Laval, 1065 Avenue de la Médecine, Québec, Canada G1V 0A6

SUMMARY

Benchmarking has been a useful tool for unbiased comparison of control strategies in wastewater treatment plants (WWTPs) in terms of effluent quality, operational cost and risk of suffering microbiology-related total suspended solids (TSS) separation problems. This chapter presents the status of extending the original Benchmark Simulation Model No 2 (BSM2) towards including greenhouse gas (GHG) emissions. A mathematical approach based on a set of comprehensive models that estimate all potential on-site and off-site sources of CO_2, CH_4 and N_2O is presented and discussed in detail. Based upon the assumptions built into the model structures, simulation results highlight the potential undesirable effects on increased GHG emissions when carrying out local energy optimization in the activated sludge section and/or energy recovery in the anaerobic digester. Although off-site CO_2 emissions may decrease in such scenarios due to either lower aeration energy requirement or higher heat and electricity production, these effects may be 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 of using integrated approaches when comparing and evaluating (plant-wide) control strategies in WWTPs for more informed operational decision-making.

Keywords: Carbon footprint, control strategies, GHG, modelling, multi-criteria evaluation, plant-wide, sustainability

TERMINOLOGY

Term	Definition
Greenhouse gas	Gas that absorbs and emits radiant energy within the thermal infrared range.
Benchmarking	Objective comparison of two items.

9.1 INTRODUCTION

The main focus in assessing the operation of wastewater treatment plants (WWTPs) has historically been the effluent water quality under constraints of technical feasibility and cost. This certainly still holds, but discussions on sustainability in general, and the impact on climate change due to greenhouse gas (GHG) emissions in particular, have widened the scope for utilities and regulators (Gustavsson & Tumlin, 2013). 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 (Mannina *et al.*, 2016; Nguyen *et al.*, 2020).

Aside from evaluating control and operational strategies (Gernaey *et al.*, 2014) before full-scale implementation (Ayesa *et al.*, 2006), dynamic activated sludge models (ASMs) (Henze *et al.*, 2000) have been widely used for multiple purposes in wastewater engineering, such as control and monitoring (Olsson 2012), benchmarking (Jeppsson *et al.*, 2007; Solon *et al.*, 2017), diagnosis (Rodriguez-Roda *et al.*, 2002), design (Flores-Alsina *et al.*, 2012), teaching (Hug *et al.*, 2009), optimization (Feldman *et al.*, 2018; Rivas *et al.*, 2008), and regulatory policy development of wastewater treatment plants (Meng *et al.*, 2016, 2020). Based on new knowledge on the chemical and biochemical mechanisms of GHG production, several efforts have been made to capture emissions of CO_2, CH_4 and N_2O, and to integrate these processes in the traditional ASMs (Domingo-Felez *et al.*, 2017; Ni & Yuan, 2015; Poquet *et al.*, 2016).

In recent years, an increasing number of studies have discussed the need for adding a new dimension related to GHG production and emission to the traditional effluent quality and operational cost indices within the performance evaluation procedures of activated sludge control strategies (Flores-Alsina *et al.*, 2011, 2014; Guo et al., 2012; Sweetapple *et al.*, 2015). In this chapter, an extended version of the International Water Association (IWA) Benchmark Simulation Model No 2 (BSM2), that is BSM2G, is used to show how decision making about the most suitable control/operational strategies may change when a GHG emission dimension is added. The model based methodology includes all major contributions to assess the carbon footprint of the plant under study. Two case studies (case study#1 and #2) are presented involving changes in the following operational 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 the sludge treatment section of the plant. Furthermore, we consider the main interactions between the water and sludge line. Finally, changes in effluent quality index (*EQI*), operational cost index (*OCI*) and CO_2, CH_4 and N_2O emissions are analysed by means of different graphical representations. As a side effect, synergies and trade-offs between local energy optimization and the overall GHG production are studied in detail.

9.2 BENCHMARK PLANT DESCRIPTION

The WWTP under study has the same layout as the IWA Benchmark Simulation Model No 2 platform proposed by Gernaey *et al.* (2014) (see Figure 9.1). The BSM2 was initially conceived for unbiased

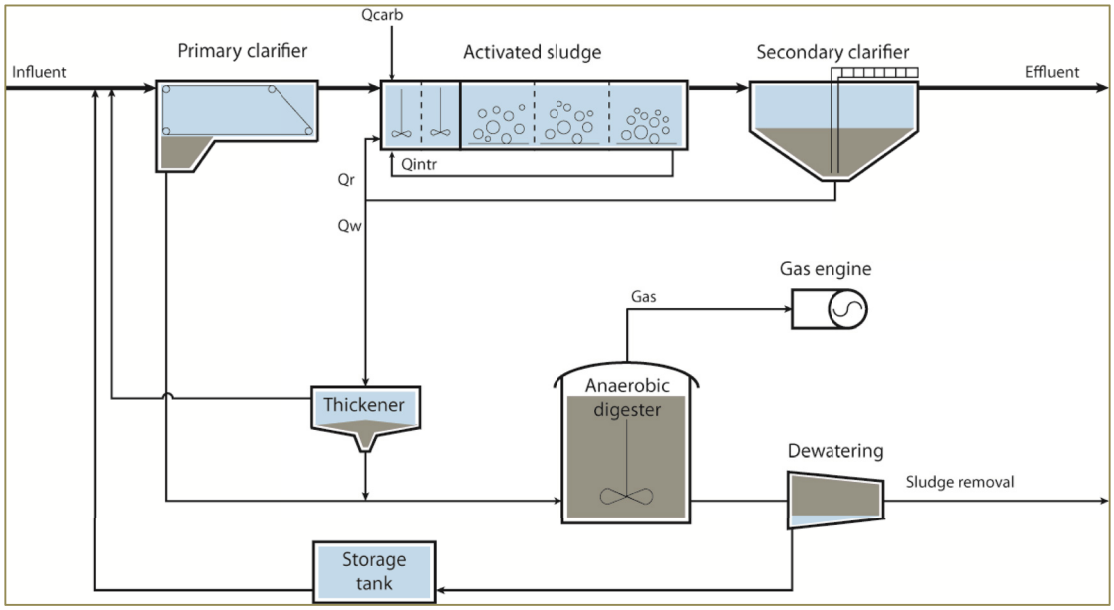

Figure 9.1 Schematic representation of the BSM2 plant layout.

comparison of control strategies based on predefined process and sensor models, influent disturbances and evaluation criteria. More specifically, the plant treats an influent flow rate of 20 648 $m^3 \cdot day^{-1}$ and total COD and N loads of 12 240 and 1 140 $kg \cdot day^{-1}$, 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 five tanks in series. Tanks 1 (ANOX1) and 2 (ANOX2) are anoxic (total volume = 3 000 m^3), while tanks 3 (AER1), 4 (AER2) and 5 (AER3) are aerobic (total volume = 9 000 m^3). AER3 and ANOX1 are linked by means of an internal recycle with the purpose of nitrate recycle for pre-denitrification. The BSM2 plant further contains a primary (PRIM, 900 m^3) and a secondary (SEC, 6 000 m^3) clarifier, a sludge thickener (THK), an anaerobic digester (AD, 3 400 m^3), a storage tank (160 m^3) and a dewatering unit (DW). Additional information about the plant design and operational conditions can be found in Gernaey *et al.* (2014).

9.3 BENCHMARK MODEL UPGRADES AND MODIFICATIONS

9.3.1 Activated sludge model (ASM)

The Activated Sludge Model No. 1 (ASM1) (Henze *et al.*, 2000) has been expanded based on 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 (FA) 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. Parameter values were adjusted according to Guo and Vanrolleghem (2014).

9.3.2 ASM/ADM interface

The interfaces presented in Nopens *et al.* (2010) have been modified to link the upgraded ASM and the default Anaerobic Digestion Model No. 1 (ADM1), by considering chemical oxygen demand (COD) and N balances for all oxidized nitrogen compounds. This is especially critical in Step 1 of the ASM–ADM interface where all negative COD (i.e. oxygen, nitrate, nitrite, nitrous oxide and nitrogen monoxide) is subtracted from the COD pool with an associated loss of substrate (S_s, X_s, X_{BH}, X_{BA} in that order). The last step, where inorganic carbon (S_{IC}) is calculated as part of the assumption of charge conservation at both sides of the interface is upgraded with the new (oxidized) nitrogen species, that is S_{NO3} and S_{NO2}. There are no modifications to the original formulation of the ADM–ASM interface.

9.3.3 Mass transfer

Mass transfer between the liquid and the gas phase in the ASM is modelled for selected compounds (S_{N2}, S_{NO} and S_{N2O}). Specific transfer coefficients (K_La_{N2}, K_La_{NO} and K_La_{N2O}) are estimated using the ratio of the squared roots of diffusivities (Foley *et al.*, 2011). The transport rates are formulated as a function of the difference between the saturation concentration and the actual concentration of the gas dissolved in the liquid (Batstone *et al.* 2012). The saturation concentration of the gas in the liquid is given by Henry's law of dissolution, which states that the saturation concentration is equal to the product of Henry's constant (K_H) multiplied by the partial pressure of the gas (P_i).

9.3.4 Temperature correction

To account for seasonal variability, liquid-gas saturation constants, kinetic parameters, transfer coefficients and equilibrium reactions are temperature dependent. More specifically, growth and decay rates are modelled according to the Ratkowsky equations. Equilibrium constants to calculate FA and FNA are adjusted using Van't Hoff corrections. Finally, K_La is kinetically adjusted with temperature changes (Gernaey *et al.*, 2014).

9.3.5 Other ancillary models

The other models have not been modified from their original description in Gernaey *et al.* (2014). The primary clarifier is modelled in accordance with Otterpohl and Freund (1992). The double exponential settling velocity function of Takács *et al.* (1991) is used to model the secondary settling process through a one-dimensional model consisting of 10 layers. Regarding the thickener and dewatering units, these are modelled as ideal, continuous processes with no biological activity, and with a constant percentage of TSS in the concentrated sludge flows leaving the thickening and dewatering units. The widely recognized ADM1 (Batstone *et al.*, 2002) is the dynamic anaerobic digestion model implemented.

9.4 EVALUATION CRITERIA

9.4.1 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, 5-day biochemical oxygen demand (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*) (Gernaey *et al.*, 2014). 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). Only the last 364 days are used for the evaluation itself.

9.4.2 On-site/off-site GHG emissions

The comprehensive approach suggested by Flores-Alsina *et al.* (2011, 2014) is used to estimate all potential GHG emissions from the studied WWTP that cannot be obtained from the explicit results of the modified BSM2. The overall GHG evaluation comprises the estimation of GHG emissions from the following sources: (i) direct secondary treatment, (ii) sludge processing, (iii) net power and chemical use, (iv) sludge disposal and reuse, and (v) receiving waters. It is important to highlight that the GHGs are converted into units of CO_2 equivalent (CO_2e) to properly deal with the different natures of the generated GHGs (CO_2, CH_4 and N_2O). Further information can be found in Flores-Alsina *et al.* (2011, 2014) and Corominas *et al.* (2012).

9.4.2.1 Direct secondary treatment emissions

Direct emissions from the activated sludge process are calculated in the bioprocess model, including CO_2 generation from microbial respiration, and production and emission of N_2O. The CO_2 is credited for growth of autotrophic nitrifying organisms with a factor of 0.31 kg CO_2/kg $N_{\text{nitrified}}$ (Tchobanoglous *et al.*, 2003). Most of the produced N_2O will be stripped to the surrounding gas phase in reactors with forced aeration and only a small fraction remains in solution. In the BSM2G, the dissolved N_2O is assumed to follow the plant effluent to the receiving waters.

9.4.2.2 Sludge processing emissions

The GHG emissions from sludge treatment are mainly generated in the anaerobic digester. Direct biogas CO_2 and CH_4 emissions are quantified using the ADM1. 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 assumed to be released to the atmosphere.

In addition, direct emissions of CO_2, CH_4 and N_2O from the sludge train of the BSM2G plant (i.e. thickener, digester, dewatering and sludge storage) are accounted for. From the AD and the gas system a leakage of 1% of the raw biogas is assumed (Avfall Sverige Utveckling, 2009). The gas flow available for utilization is therefore reduced by the corresponding amount. The CH_4 that remains dissolved in the sludge after digestion is assumed to be stripped at the dewatering unit and adds to the emissions.

Based on common practice in countries applying dewatered sludge as fertilizer on productive land (e.g. crops or forest), it is assumed that the sludge is stored uncovered at the plant for 12 months (for hygienic purposes) before use. During storage, post digestion occurs, leading to GHG emissions. The emissions of CH_4 and N_2O are set to 8.7 g CH_4/kg volatile solids (VS) and 0.36% of total nitrogen (TN) as N_2O-N (Jönsson *et al.*, 2015). Corresponding amounts of carbon and nitrogen are subtracted from the sludge (S_S, X_S and S_{NH}).

In the gas engine, the CH_4 in the biogas is combusted and converted to CO_2 which is emitted with the fumes along with a fraction of the gas that passes through the engine un-combusted. The emission factor (EF) for un-combusted biogas is set to 1.7% of the gas fed to the gas engine (Liebetrau *et al.*, 2010). Consequently, the energy production is reduced by the same factor.

9.4.2.3 Net power and chemical use emissions

Net energy is calculated as the difference between energy consumption (aeration, pumping, mixing and heating) and energy production. The electricity generated by the turbine is calculated by using a factor for the energy content of the methane gas (50 014 MJ/kg CH_4) and assuming a 43% efficiency for electricity generation. For external electricity required, a value of 0.359 kg CO_2e/kWh is assumed (Arnell *et al.*, 2017).

It is assumed that methanol is used as external carbon source for denitrification. A common type of methanol, sourced from fossil resources, is assumed with an emission factor of 1.54 kg CO_{2e}/kg MeOH. Methanol is the only chemical included in the BSM2G (Dong & Steinberg, 1997).

9.4.2.4 Sludge disposal and reuse emissions

After 12 months of storage, the sludge is transported for final disposal or reuse. While reuse options, transport distance and specific emissions vary widely with location, the following mix of disposal options is chosen (Arnell *et al.*, 2017):

(i) Crop land – 38% of the sludge; 150 km transport; N_2O Emission Factor (EF): 0.01 kg N_2O-N/kg TN.
(ii) Composting – 45% of the sludge; 20 km transport; N_2O EF: 0.01 kg N_2O-N/kg TN CH_4 EF: 0.0075 kg CH_4/kg total organic carbon (TOC)
(iii) Forest – 17% of the sludge; 144 km transport; N_2O EF: 0.01 kg N_2O-N/kg TN

GHG emissions resulting from transport of sludge are calculated with an emission factor for Euro 4 class trucks running on diesel for all disposal options, where unloaded return trips are assumed.

9.4.2.5 Receiving water emissions

Indirect emissions of N_2O from the recipient due to residual nitrogen in the effluent are calculated and presented (Arnell *et al.*, 2017). Studies of N_2O emissions from natural waters show a large variability depending on climate and type of water system (lake, river, sea, etc.). For BSM2G, an emission factor corresponding to an inland lake or river was included, 0.0003 kg N_2O-N/kg $TN_{effluent}$ (IPCC, 2013).

9.4.3 Sustainability indicators

Additional indicators can be calculated for economic and environmental aspects of sustainability – these are inspired by the work of Molinos-Senante *et al.* (2014) and detailed fully by Sweetapple *et al.* (2014a, 2015). Societal aspects are not considered since typical indicators (such as noise, odour and visual impact) cannot be determined from the model, and are not expected to be subject to any perceivable change as a result of adjusting control strategies.

Operational costs, represented by the *OCI*, are considered within economic sustainability. Capital/investment costs associated with implementation of a new control strategy cannot be quantified from the model, but are expected to be small relative to the long-term operational costs.

Environmental sustainability is assessed based on (i) treatment efficiency, (ii) net energy consumption, (iii) sludge production, and (iv) GHG emissions. The percentage of influent COD, TSS and total nitrogen removed (or not removed), based on the modelled influent and effluent concentrations, provide three indicators for treatment efficiency. Net energy consumption is quantified as in the calculation of GHG emissions, based on energy uses included in the *OCI* and credit from the energy content of recovered methane (Section 9.4.2). Sludge production is calculated as in the *OCI* (Gernaey *et al.*, 2014), and emissions from secondary treatment, sludge processing, net power, chemical use and sludge disposal and reuse are included in the calculation of total GHG emissions, as detailed in Section 9.4.2.

9.5 EXAMPLES/CASE STUDIES

9.5.1 Case study #1: evaluation of plant-wide control strategies

In the first case study, the BSM2G is simulated in a closed loop regime, which includes two defined proportional integral (PI) control loops. The first loop controls the dissolved oxygen (DO) concentration in AER2 by manipulating the air supply rate, here implemented as the oxygen transfer coefficient K_La4 (set-point = 2 g $O_2 \cdot m^{-3}$). 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 temperature (above or below 15°C) 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 control scenarios are simulated in the previously predefined case study:

(i) *Impact of DO control* (commonly used to reduce aeration costs) by varying the set-point value between 1 and 3 g $O_2 \cdot m^{-3}$ (default value 2 g $O_2 \cdot m^{-3}$).
(ii) *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.
(iii) *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).
(iv) *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 experiencing high load) and returns it at night (when the plant is at low load). Note that the default BSM2 strategy does not use this control approach and liquors from dewatering are simply returned as they are generated.

EQI, *OCI* and GHG values for the different simulated scenarios are shown in Figure 9.2. Hence, it is possible to see how the overall picture changes when: (i) *EQI* and *OCI* are considered only (Figure 9.2a, b); or (ii) when adding the total quantity of CO_2, N_2O and CH_4 emissions (quantified in kg CO_2e. m^{-3} of treated wastewater) (Figure 9.2c, d). From the generated results one can see that: (i) the DO set-point in the activated sludge section is of paramount importance to the plant's total GHG emissions (*z*-axis) next to the well-known impacts on effluent quality and operating costs; (ii) better TSS removal efficiency in PRIM mainly improves effluent quality and operational cost (*x*- and *y*-axis), but the total GHG emissions remain almost equal; (iii) 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; and (iv) control of the anaerobic digester supernatants return flow rate improves effluent quality, slightly increases cost but does not have an effect on the GHG emissions unless DO is very low (see dotted lines in Figure 9.2b).

The study presents an important result to the wastewater community by demonstrating the potential impacts of *energy optimization*, particularly in the aeration/anaerobic digester system, and by showing the importance of *plant-wide evaluation*. For example, based on the reported 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 Figure 9.2a, b). The situation becomes even worse when GHG emissions are included in the analysis (Figure 9.2c, d) and the substantial contribution of N_2O in the total plant's global warming potential would rank that alternative even lower. Another example in Figure 9.2 illustrates the potential of improving the % TSS removal in the PRIM. Firstly, the load to the activated sludge section is substantially reduced (and thus the off-site CO_2 emissions due to aeration) when the % TSS removal in PRIM increases. Secondly, there is an increase in energy recovery from the anaerobic digestion (higher CO_2 credit). However, in terms of total quantity of GHG emissions the strategy does not seem to pay off since there is a substantial increase in N_2O emissions due to the inadequate C/N ratios that result (poor denitrification). These two examples demonstrate the usefulness of a third GHG dimension for deciding on the optimum operational setting to meet a specific plant's objectives.

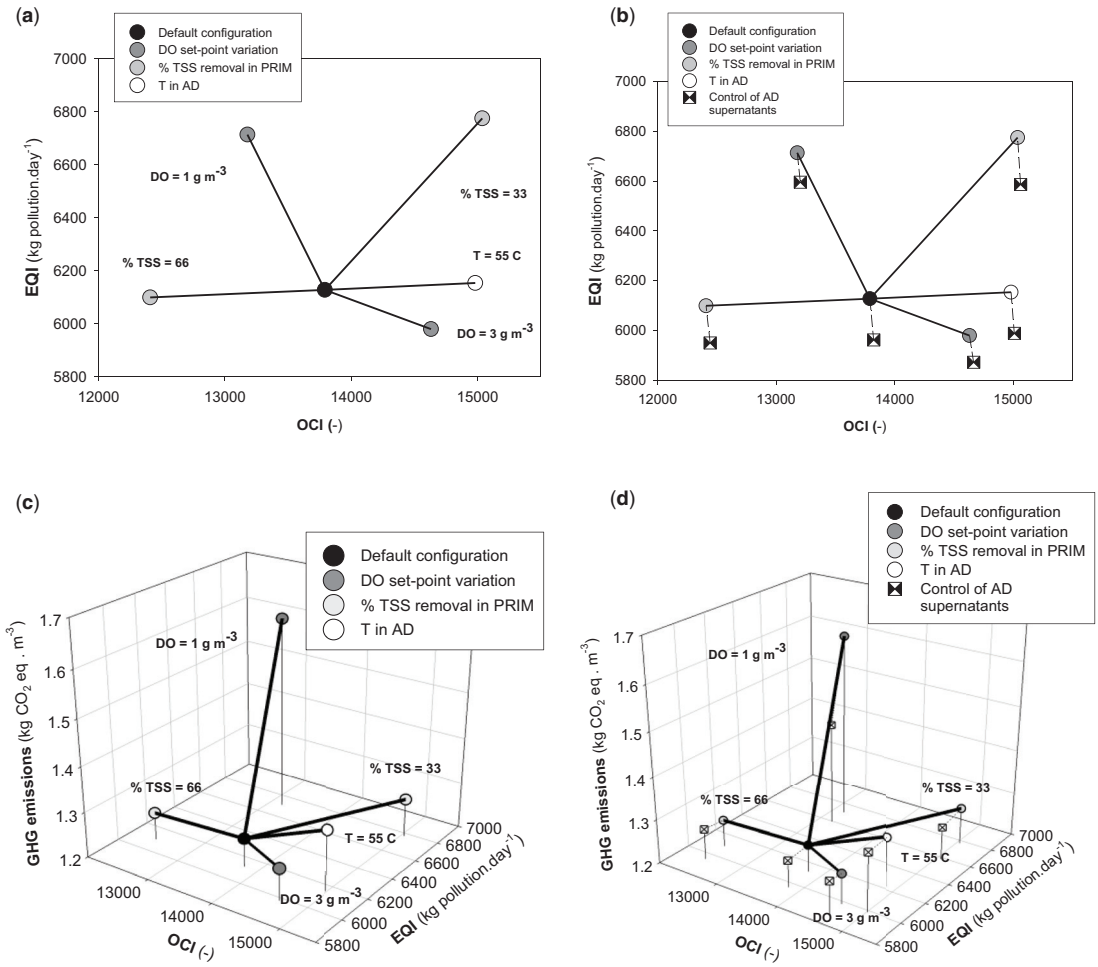

Figure 9.2 Effluent, cost and emission criteria for all the evaluated strategies. (a), (b) *EQI* & *OCI*, (c), (d) *EQI*, *OCI* & *GHG*.

9.5.2 Case study #2: investigating the impact of net energy reduction on sustainability

This case study aims to more broadly investigate the effect on sustainability of modifying the plant control system to reduce net energy use. It considers both economic and environmental aspects of sustainability (including GHG emissions), using the indicators presented in Section 9.4.3.

Two different control strategies are considered, each with multiple variants. In the first control strategy (CL1), DO is controlled using a single PI control loop, as described for Case Study #1. In the second (CL2), three independent PI control loops are used to control the DO spatial distribution, with oxygen transfer coefficients K_La3, K_La4 and K_La5 manipulated to control the DO concentration in AER1, AER2 and AER3 respectively (based on previous findings by Jeppsson *et al.* (2007) that this uses less energy for aeration than a range of other alternatives). In both control strategies, an additional PI control loop controls the nitrate concentration in ANOX2 by manipulating the internal recycle flow rate and different waste sludge flow rates are imposed depending on the time of year. This controller was not included in case study #1.

Factorial sampling is used to generate sets of waste sludge flow rates and DO set-points to implement in these control strategies (within the range 240–360 $m^3 \cdot day^{-1}$ for winter waste sludge flow rate, 360–540 $m^3 \cdot day^{-1}$ for summer waste sludge flow rate, 1–3 g $O_2 \cdot m^{-3}$ for the DO set-point in CL1, and 0.5–2.0 g $O_2 \cdot m^{-3}$ for the DO set-point in CL2). This provides a total of 315 control options for evaluation. CL1 with waste sludge flow rates and DO set-point as in Case Study #1 represents the base case option. Further details on the control options can be found in Sweetapple *et al.* (2015).

A pair-wise comparison of sustainability indicators for control options which provide a reduction in net energy (with respect to the base case) and a compliant effluent is shown in Figure 9.3. Whilst

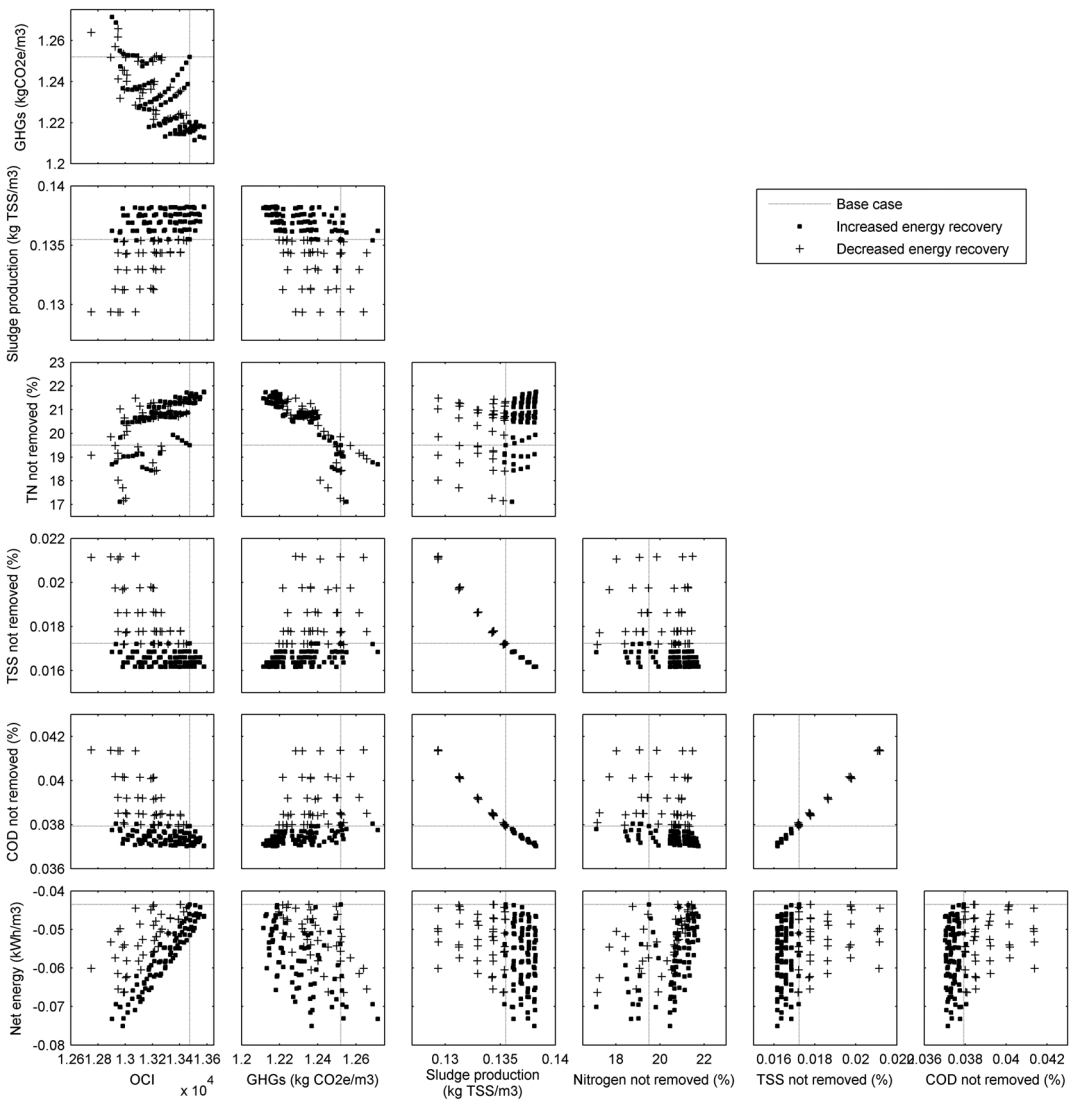

Figure 9.3 Sustainability indicator values for control options providing a reduction in net energy and a compliant effluent.

this shows that control options selected to reduce net energy use also reduce GHG emissions in a high proportion of cases, it also highlights that increased GHG emissions are a potential adverse side effect (as observed in 10% of cases). This may be attributed to lower DO set-points providing lower energy consumption but increased N_2O formation (Flores-Alsina *et al.*, 2014), and raises the important issue that reducing energy use cannot be seen as a reliable approach for reducing total GHG emissions. These results also show that few of the considered solutions (11%) both maintain/improve nitrogen removal and reduce GHG emissions. This highlights a particular challenge since N_2O is emitted during nitrification and denitrification and, whilst these emissions can be curbed to some extent by ensuring sufficient DO (Kampschreur *et al.*, 2009), this will have implications on energy use.

The best solution with respect to energy reduction is the CL2 control strategy with a 20% increase in the waste flow rates and DO set-points of 1, 1, and 0.5 g $O_2 \cdot m^{-3}$ in AER1, AER2 and AER3 respectively, which uses 73% less energy than the base case. However, this does not provide a universal improvement in sustainability, with both nitrogen removal and sludge production worsened. None of the control options evaluated in fact provides an improvement in all of the sustainability indicators, although seven provide an improvement in all but one. The performance of these control options, alongside the solution that provides the minimum net energy use are shown in Figure 9.4.

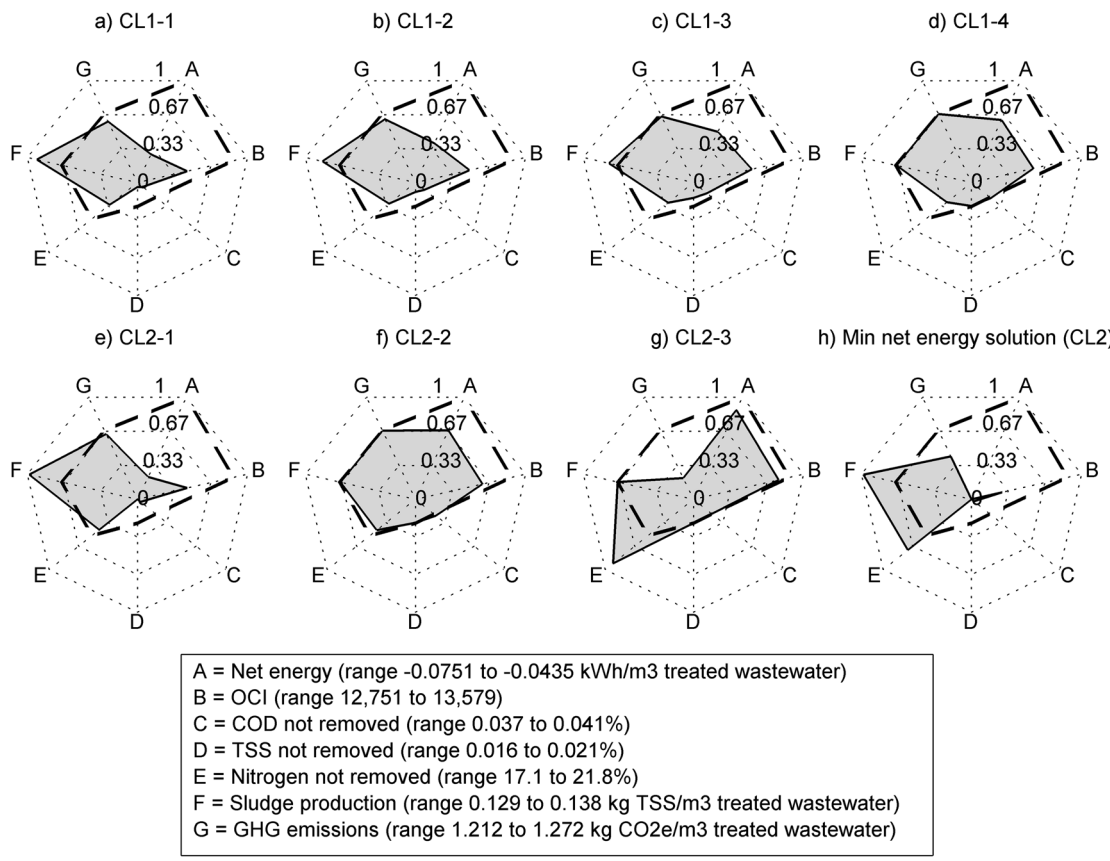

Figure 9.4 Sustainability indicator values for selected solutions, with the dashed lines representing the base case and values closer to the centre of the plot being preferable. (a) CL1-1, (b) CL1-2, (c) CL1-3, (d) CL1-4, (e) CL2-1, (f) CL2-2, (g) CL2-3, (h) Min net energy solution (CL2).

This illustrates that, although each solution reduces net energy use, the type and magnitude of their sustainability impacts vary considerably and trade-offs must be considered.

The results of this case study are of importance because they highlight that, whilst improving both DO control and waste flow rate selection can provide substantial energy savings and increase economic sustainability, the impacts on environmental sustainability are not universally beneficial. Trade-offs are identified and it is shown that nitrogen removal and sludge production in particular are likely to be detrimentally affected in the lowest energy solutions. The ability to model and include both on-site and off-site GHG emissions is particularly valuable since solutions are identified in which a significant reduction in net energy corresponds with an increase in total GHG emissions; in the absence of emissions modelling, such solutions might be assumed to have a more beneficial environmental impact than is the case in reality.

9.5.3 Other relevant case studies

Besides case study #1 and #2 presented in this chapter, there have been many other investigations where the BSM2G has been applied to evaluate control strategies with different purposes, for example, the evaluation of control strategies in further studies using multi-objective optimization (Sweetapple *et al.*, 2015). Control strategies have also been developed which are particularly focused on reducing N_2O emissions (Boiocchi *et al.*, 2017a, 2017b; Santin *et al.*, 2017). It is important to mention the different types of sensitivity analysis that have been implemented in the platform in order to gain understanding of the main interactions amongst model parameters (Boiocchi *et al.*, 2017b; Sweetapple *et al.*, 2014b). Finally, the original WWTP layout has been modified by including sewer and catchment models to also account for CH_4 emissions within the sewer network (Guo *et al.*, 2012). Additional modifications consist of adding two extra anaerobic tanks to allow for biological phosphorus removal (Solis *et al.*, 2019).

9.6 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.*, 2016). In this paper, the N_2O production by AOB is based on denitrification with NH_4^+ as the 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 (Wunderlin *et al.*, 2013). Recent investigations demonstrate that both the autotrophic denitrification and the NH_2OH oxidation are involved in N_2O production, although the latter to only a minor degree (Domingo-Felez *et al.*, 2017; Ni & Yuan, 2015; Poquet *et al.*, 2016). Therefore, the results reflect the assumptions built into the N_2O model structure of Mampaey *et al.* (2013), and Guo and Vanrolleghem (2014).

The recent advances when modelling physicochemical processes (Batstone *et al.*, 2012; Flores-Alsina *et al.*, 2015) would allow: (i) pH calculation according to influent conditions and process conditions; and (ii) FA and FNA calculation accounting for ion strength and ion pairing. Indeed, several investigations showed the substantial impact that weak acid chemistry might have on N_2O emissions (Su *et al.*, 2019). Another important aspect would be the quantification of biogenic CO_2 emissions and their inclusion in the overall carbon balance within the plant. Preliminary results can be found in Solis *et al.* (2022).

9.7 CONCLUSIONS AND PERSPECTIVES

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 global warming potential (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 are controlled.
- While these observations are WWTP specific, the use of the developed tools is demonstrated and can be applied to other systems.

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NOMENCLATURE

AD	Anaerobic digester
ADM	Anaerobic digestion model
AE	Aeration energy (kWh·day^{-1})
AER	Aerobic section
AOB	Ammonium oxidizing bacteria
ANOX	Anoxic section
ASM	Activated sludge model
BOD	Biochemical oxygen demand (g·m^{-3})
BSM2	Benchmark Simulation Model No 2
CH_4	Methane (kg CH_4·day^{-1})
CO_2	Carbon dioxide (kg CO_2·day^{-1})
CO_2e	Equivalent carbon dioxide (kg CO_{2e}·day^{-1})
COD	Chemical oxygen demand (g·m^{-3})
DO	Dissolved oxygen concentration (g·m^{-3})
DW	Dewatering unit
EC	Consumption of external carbon source (kg COD·day^{-1})
EQI	Effluent quality index (kg pollution·day^{-1})
GHG	Greenhouse gas
GWP	Global warming potential
HE	Heating energy (kWh·day^{-1})
K_La	Volumetric oxygen transfer coefficient (day^{-1})
ME	Mixing energy (kWh·day^{-1})
MP	Methane production (kgCH_4·day^{-1})
N	Nitrogen
NH_4^+	Ammonium nitrogen (g N·m^{-3})
NO	Nitric oxide nitrogen (g N·m^{-3})
N_2O	Nitrous oxide nitrogen (kg N·day^{-1})
NOB	Nitrite oxidizing bacteria
NO_2^-	Nitrite nitrogen (g N·m^{-3})
NO_3^-	Nitrate nitrogen (g N·m^{-3})
NO	Oxidized forms of nitrogen (g N m^{-3})
OCI	Operational cost index (-)
PE	Pumping energy (kWh·day^{-1})

PRIM	Primary clarifier
PI	Proportional integral controller
Q_e	Effluent flow rate ($m^3 \cdot day^{-1}$)
Q_{carb}	External carbon source 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·day^{-1})
ST	Storage tank
SRT	Sludge retention time (days)
TKN	Total Kjeldahl nitrogen ($g \cdot m^{-3}$)
TN	Total nitrogen ($g \cdot m^{-3}$)
THK	Thickener
TOC	Total organic carbon ($g \cdot m^{-3}$)
TSS	Total suspended solids ($g \cdot m^{-3}$)
VS	Volatile solids ($g \cdot m^{-3}$)
WWTP	Wastewater treatment plant