Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment

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\textbf{ABSTRACT}

This research investigates the effects of adjusting control handle values on greenhouse gas emissions from wastewater treatment, and reveals critical control handles and sensitive emission sources for control through the combined use of local and global sensitivity analysis methods. The direction of change in emissions, effluent quality and operational cost resulting from variation of control handles individually is determined using one-factor-at-a-time sensitivity analysis, and corresponding trade-offs are identified. The contribution of each control handle to variance in model outputs, taking into account the effects of interactions, is then explored using a variance-based sensitivity analysis method, i.e., Sobol’s method, and significant second order interactions are discovered. This knowledge will assist future control strategy

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development and aid an efficient design and optimisation process, as it provides a better understanding of the effects of control handles on key performance indicators and identifies those for which dynamic control has the greatest potential benefits. Sources with the greatest variance in emissions, and therefore the greatest need to monitor, are also identified. It is found that variance in total emissions is predominantly due to changes in direct $N_2O$ emissions and selection of suitable values for wastage flow rate and aeration intensity in the final activated sludge reactor is of key importance. To improve effluent quality, costs and/or emissions, it is necessary to consider the effects of adjusting multiple control handles simultaneously and determine the optimum trade-off.

*Keywords*: Greenhouse gas; wastewater treatment; operation; control; sensitivity

1 INTRODUCTION

Developing strategies for the reduction of greenhouse gas (GHG) emissions is a topic of great interest and current relevance, as countries have committed to emission reduction targets under the Kyoto Protocol to mitigate the effects of global warming. Energy use in the water industry is an important source of GHG emissions; whilst in Europe it only typically contributes 1% of national consumption, this is predicted to increase (Olsson, 2012), and in the U.S.A. 4% of
electricity demand is attributable to the movement and
treatment of water and wastewater (Mo et al., 2010).

Wastewater treatment also results in the formation and direct
emission of the GHGs carbon dioxide (CO₂), methane (CH₄)
and nitrous oxide (N₂O). The wastewater sector was
responsible for over 5% of global non-CO₂ GHG emissions in
2005, and these emissions are predicted to increase by 27% by
2030 (U.S. Environmental Protection Agency, 2012).

Wastewater utilities must contribute to emission reduction
targets, but are faced with the challenge of simultaneously
improving effluent quality and managing costs.

Appropriate operation of wastewater treatment processes can
play a significant role in reducing GHG emissions (Gori et al.,
2011) and wastewater treatment plant (WWTP) control
strategies which both improve effluent quality and reduce GHG
emissions have been developed (Flores-Alsina et al., 2011; Guo
et al., 2012). However, control handles with the greatest impact
on GHG emissions need to be identified if significant further
improvements are to be made. The effects of adjusting the
dissolved oxygen (DO) setpoint, sludge retention time (by
alteration of the wastage flow rate), carbon source addition rate,
primary clarifier TSS removal efficiency, anaerobic digester
temperature and control of the digester supernatant return flow
on GHG emissions from different sources, as well as effluent
quality and operational cost, have been assessed previously
Since the effects of interactions due to simultaneous adjustments or strategy implementations were not considered and variation within the full range of feasible values not explored, however, key findings regarding the effects of these adjustments are of limited use in further control strategy development. The importance of analysing a wide range of values for each control handle is evidenced by the identification of non-linear relationships between parameter values and effluent quality, and control handle values beyond which further increase produces no additional gain (Nopens et al., 2007). Previous analysis (Benedetti et al., 2012) has identified control handles to which effluent quality and operational cost are most sensitive in the Benchmark Simulation Model No. 2 (BSM2) (Jeppsson et al., 2007), taking into account simultaneous variation across a range of values, but the impacts on GHG emissions have not been considered. Furthermore, whilst the effects of interactions are automatically considered when multiple control changes are implemented, the relative significance of specific interactions between control handles cannot be revealed explicitly to inform control strategy development by focusing on interactions. It would also be beneficial to investigate variance in GHG emissions from different sources, in order that control strategy development can focus on those with greatest potential for improvement. For example, manufacture of material for on-site
usage is a key source of GHG emissions (Shahabadi et al., 2010) but, given that previous studies show little variation in emissions resulting from chemical consumption under different control strategies (Guo et al., 2012), attempts to reduce GHG emissions by reduction of carbon source addition may be ineffective without introduction of alternative treatment processes such as Anammox. Conversely, it has been found that implementation of different control strategies can result in significant variation in the magnitude of N$_2$O emissions from activated sludge (Guo et al., 2012), suggesting that there is great potential for reduction of total GHG emissions from wastewater treatment by reducing N$_2$O emissions. It is known that DO concentration and COD/N ratios, which are controlled by adjustment of aeration and carbon source addition rates, play a key role in controlling production of N$_2$O (Kampschreur et al., 2009; Guo et al., 2012), yet there is a need to investigate the effects on net emissions of varying these control handles simultaneously, as well as the effluent quality and operational cost. At present, there are conflicting observations regarding the effects of WWTP control on N$_2$O emissions: Clippeleir et al. (2014), for example, measured increased N$_2$O emissions when operating with a high DO setpoint, whilst Guo et al. (2012) found a reduction in DO setpoint to correspond with an increase in N$_2$O emissions.
This research aims to detect control handles to which key performance indicators (including GHG emissions, effluent quality and operational cost) are sensitive and to identify the most significant sources of variance in total GHG emissions, taking into account interaction effects. It is important to identify control handles to which GHG emissions are significantly more sensitive than effluent quality or operational costs, since selection of their values might be attributed little importance in conventional design practices. This knowledge will guide the selection of control handles for efficient and effective control strategy development, based on those with potential to yield the greatest improvements. Knowledge of control handles to which no key model outputs are sensitive will also reduce the number of decision variables required, therefore reducing computational demand and improving the feasibility of multi-objective optimisation for control strategy development.

Sensitivity analysis is employed to identify important parameters controlling model outputs (Tang et al., 2007a); this approach can be utilised to assist system optimisation by detecting the most influential control handle(s) (Naessens et al., 2012), and has previously been shown to be effective (Fu et al., 2012). Analysis is carried out through the combined use of a local sensitivity method - one-factor-at-a-time (OAT) - and a variance-based global method – Sobol’s method; this allows
trade-offs to be investigated, and reveals control handles with significant individual effects on GHG emissions, effluent quality and operational cost, as well as those with interaction effects which contribute significantly to variance in the model outputs. Model evaluations carried out with global sensitivity analysis (GSA) also reveal the most significant sources of variance in GHG emissions and, therefore, the sources from which it is most important to control and monitor GHG emissions.

2 MATERIALS AND METHODS

2.1 Wastewater treatment plant description and modelling

Wastewater treatment processes are simulated in this work using BSM2-e (Sweetapple et al., 2013), a WWTP model based on the BSM2 (Jeppsson et al., 2007) but with modifications made to enable dynamic modelling of GHG emissions (Sweetapple et al., 2013). The plant consists of a primary clarifier, an activated sludge unit containing five tanks in series (two anoxic followed by three aerobic), a secondary settler, a sludge thickener, an anaerobic digester and a dewatering unit. Control handles included in this analysis are restricted to 14 available in BSM2 (shown in Figure S1): aeration and carbon source addition rates in each of the five reactors ($KLa1\text{-}5$ and $carb1\text{-}5$), internal recirculation flow rate ($Qintr$), return sludge
flow rate \( (Q_r) \), wastage flow rate \( (Q_w) \) and reject water flow rate setpoint \( (Q_{storage}) \). \( Q_r \) and \( Q_w \) are included despite previously having been found not to have a significant effect on effluent quality and operational cost (Benedetti et al., 2008), since their interactions with other control handles were not previously investigated, their effects on GHG emissions are unknown, and the range of \( Q_w \) values considered was insufficient to encompass those previously proposed for operation of BSM2 (Nopens et al., 2010). It is also known that wastage flow rate affects aeration requirements and sludge production, both of which contribute significantly to operational costs.

The median value for each control handles is assumed to equal the BSM2 open loop default, and minimum and maximum feasible values are specified in the BSM2 code (Nopens et al., 2010). However, whilst a large range of values are possible, it might not be realistic in practice to operate the WWTP with some or all of the control handles at the extremes of their allowable ranges. Therefore, for the purposes of sensitivity analysis, upper and lower bounds are set to the default value \( \pm 10\% \) of the allowable range (with the lower limit set to zero where this gives a negative number).

GHG emissions are modelled as detailed by Sweetapple et al. (2013). Sources of direct GHG emissions include \( \text{CO}_2 \) and \( \text{N}_2\text{O} \) from substrate utilisation, biomass decay and incomplete
denitrification in the activated sludge reactors, leakage and/or combustion of \( \text{CO}_2 \) and \( \text{CH}_4 \) from the anaerobic digester, and \( \text{CH}_4 \) stripped from solution in the dewatering unit. Indirect emissions resulting from generation of net energy imported, manufacture of chemicals used, degradation of effluent, and sludge transportation and degradation are also modelled.

Additional \( \text{CH}_4 \) emissions, which may result from unintentionally anaerobic conditions (Monteith et al., 2005), are not modelled due to a lack of reliable estimation techniques. \( \text{N}_2\text{O} \) emissions from nitrifier denitrification during nitrification are also omitted due to a lack of suitable modelling techniques – metabolic models exist (Ni et al., 2011; Mampaey et al., 2013) but have been found unable to accurately and consistently reproduce experimental data (Law et al., 2012; Ni et al., 2013; Sperandio et al., 2014). The significance of these omissions is uncertain, as previous field studies have identified \( \text{CH}_4 \) emissions from every processing unit (Wang et al., 2011) and nitrifier denitrification is known to yield high \( \text{N}_2\text{O} \) emissions relative to the mass of nitrogen emissions converted, although the proportion of nitrogen removal attributed to this pathway is hard to determine (Kampschreur et al., 2009). If these sources are included in future GHG emission estimates for control strategy development, further work to investigate their variance resulting from the choice of control handle values is recommended.
Further details on the control handles included in this analysis are provided in the supplementary information.

2.2 Preliminary investigation using OAT

Preliminary investigation is carried out using OAT sensitivity analysis, which allows changes in model outputs to be attributed to a specific control handle, with no ambiguity: two WWTP performance evaluations are carried out for each control handle (one with the value at its lower bound and another with the value at its upper bound, whilst all other control handles are held at their default value) and the percentage change in each model output with respect to the base case is calculated. The results are then used to identify control handles with the highest control authority, and to determine the direction of change in each model output resulting from an increase or decrease in control handle value.

2.3 Global sensitivity analysis of control handles

Sobol’s method (2001) is selected for GSA, as it enables the impacts of interactions between specific control handles pairs, as well as those of individual control handles and higher order interactions, on key model outputs to be distinguished. It is more effective at identifying interactions between variables in highly non-linear models than alternatives such as analysis of variance, gives a more detailed description of the effects of
individual control handles and their interactions, and provides more robust sensitivity rankings (Tang et al., 2007b).

Sobol’s method is variance-based and centres upon the decomposition of total variance in a model output into components resulting from specific control handles and control handle interactions; Sobol’s sensitivity indices of different orders are then a measure of the output’s sensitivity to each individual control handle or control handle interaction. In this study, first and total order indices are calculated for each individual control handle and second order indices for each control handle pair. Total order indices \( S_T \) represent the percentage contribution of control handle \( i \) to output variance, taking into account the effects of interactions of all orders. Second order indices \( S_{ij} \) represent the contribution of interaction between control handles \( i \) and \( j \) only, and first order indices \( S_i \) the effects of control handles \( i \) alone. A high total order sensitivity index, therefore, indicates a control handle whose adjustment can affect model outputs significantly, and if the corresponding first order index is low, the contribution to output variance is predominantly due to interaction effects.

To implement Sobol’s method, random control handle samples are generated and WWTP performance evaluated using each set of values in turn. The total variance of each model output is calculated, and the first, second and total order sensitivity indices for each control handle or control handle pair and their
corresponding 95% bootstrap confidence intervals are computed as detailed by Tang et al. (2007b). Further details on control handle sampling are provided in the supplementary information Section 1.3.

2.4 Simulation strategy and performance assessment

The importance of developing GHG emission mitigation strategies based on dynamic simulations has been highlighted previously (Corominas et al., 2012; Guo et al., 2012), and significant differences in N₂O emissions modelled under steady-state and dynamic conditions have been identified (Guo et al., 2012). Sensitivity analysis, therefore, uses dynamic simulations to calculate key performance indicators. Performance assessment for OAT sensitivity analysis is based on a one-year evaluation period, using the BSM2 simulation strategy and influent data. However, given the high computational demand of extended simulations and the number of evaluations required, a reduced simulation period is used for GSA. This consists of 200 days of constant influent to allow the system to reach steady state, followed by 56 days of dynamic influent, of which the final 14 are used for performance evaluation. Although not fully replicating model outputs from the full length simulation (since the model may not reach quasi steady state with the reduced period of dynamic influent preceding the evaluation, and performance will differ throughout the year), this was found to be sufficient for
assessing the relative importance of each control handle in terms of their effects on each output. Further details on the choice of simulation strategy are available in the supplementary information.

Use of a shortened evaluation period provides additional benefits: if change in a specific control handle can have opposite effects depending on the state of the system (e.g. due to interaction with temperature), the resultant variance in mean performance over an extended period may be small, despite the control handle potentially being of importance. Such control handles are less likely to be overlooked with a short evaluation period and are of great interest since their dynamic control could be particularly advantageous. For sensitive control handles it is still important that potentially differing effects throughout the year are considered in control strategy development, however, since assumption that their behaviour remains as reported in this study could lead to process control related problems.

Average total GHG emissions per unit of wastewater treated are calculated to enable identification of control handles with the greatest overall effects on GHG emissions. Emissions of each individual gas from each individual source are also calculated, to allow more in-depth investigation into the greatest sources of variability and identification of critical sources. Emissions are expressed in units of CO₂ equivalent
(CO₂e) to take into account the differing effects of each GHG on global warming and enable the relative significance of emissions from different sources to be assessed. Global warming potentials of 21 g CO₂e/g CH₄ and 310 g CO₂e/g N₂O (IPCC, 1996) are used for CH₄ and N₂O respectively.

Given that design of a WWTP control strategy must also ensure that an acceptable effluent quality is achieved at a reasonable cost, performance is assessed using an effluent quality index (EQI) and an operational cost index, as defined by Jeppsson et al. (2007). The EQI is a weighted measure of the effluent loads of compounds with major effects on receiving water quality; the OCI is a measure of average energy use, energy recovery from biogas combustion, chemical usage and production of sludge for disposal.

3 RESULTS AND DISCUSSION

3.1 Impacts of adjusting control handles individually

The results of OAT sensitivity analysis of the control handles with respect to EQI, OCI and total GHG emissions are presented in Tornado diagrams (Figure 1). The percentage changes in each model output with respect to the base case, resulting from adjustment of each control handle to its upper and lower bounds individually, are shown and effects of increasing and decreasing control handle values are distinguished.
It is shown that considering the effects on GHG emissions when developing control strategies to improve effluent quality and/or reduce cost is vital, since trade-offs are identifiable and, in some instances (such as $KLa_1$ and $KLa_2$), small changes in EQI and/or OCI resulting from the first order effects of adjusting a control handle correspond with a significant change in GHG emissions.

OAT sensitivity analysis suggests that GHG emissions are affected predominantly by aeration intensities and that increasing aeration in any of the reactors would result in an increase in emissions with respect to the base case. On average, 101% of this observed increase in net total GHG emissions is attributed to increases in direct $N_2O$ emissions: this is as expected since high DO concentrations due to over aeration contribute to high $N_2O$ emissions during denitrification (Kampschreur et al., 2009) and $N_2O$ has a high GWP. Reducing aeration intensities $KLa_3$, $KLa_4$, and $KLa_5$ significantly reduces GHG emissions; however, there is a trade-off between performance indicators, and EQI is increased by over 35%.

The greatest change in total GHG emissions (32%) is achieved when $KLa_1$ is set to its upper bound. This knowledge may not enable development of improved control strategies, since adjustment of $KLa_1$ is shown only to worsen all three key
performance indicators, but the fact that adjustment of $KLa1$ has such a significant impact on GHG emissions compared with that on EQI and OCI highlights the importance of selecting suitable aeration intensities when developing control strategies. It may not be reasonable to actually operate the WWTP with control handles at the values tested, as satisfactory effluent quality would not be achieved – for example, $KLa1$ is typically set to zero since the first reactor is anoxic, but an increase would introduce aerobic conditions and severely reduce the denitrification capacity of the plant. Decreasing aeration rates in the aerobic reactors to reduce emissions could also substantially increase the EQI. The relative significance of each control handle in terms of each model output may differ when varied only within a range that provides an acceptable level of treatment. However, trade-offs must be considered and in some cases, although undesirable, it may be that a deliberate reduction in nitrogen removal is a possible means of reducing emissions in an affordable manner.

EQI and OCI are affected most significantly by $Q_w$: reducing $Q_w$ to its lower bound (giving a SRT of 46 days, within the range of an extended aeration system) results in an 85% increase in EQI and an 18% reduction in OCI. It is only ranked 6th based on its impact on GHG emissions, but a decrease in emissions corresponds with a decrease in OCI, suggesting that the most cost effective choice of flow rate to achieve the
required effluent quality will also perform favourably in terms of GHG emissions. Change in energy consumption associated with pumping provides negligible (<0.2%) contribution to the observed net change in emissions resulting from decreased $Q_w$, whilst direct emissions from activated sludge and the digester contribute 58% and 32% respectively. It is not, however, proposed that $Q_w$ be decreased to the extent modelled here, due to the significant adverse effects on effluent quality.

Adjustment of carbon source addition rates may offer potential for reducing GHG emissions, based only on their individual effects – it is known that a low COD/N ratio can increase N$_2$O emissions from denitrification (Shahabadi et al., 2009), and it is found that increasing $carb1$ or $carb2$ to their upper bound value results in a 4.9% reduction in GHG emissions with negligible (up to 0.8%) trade-off in EQI. This is, however, at the expense of OCI, which increases by 7.0% (predominantly due to costs of providing the additional carbon). No single control handle can be adjusted to improve all three performance indicators simultaneously, reinforcing the importance of considering interaction effects in control strategy development and suggesting that trade-offs may be necessary.

3.2 Relative significance of first, second and total order effects of control handles
Control handles are classified as ‘highly sensitive’, ‘sensitive’ or ‘not sensitive’ based on their first, second and total order contributions to output variance: a sensitivity index greater than 0.1 (i.e. a contribution of at least 10%) denotes a highly sensitive control handle and a sensitivity index greater than 0.05 (i.e. a contribution of at least 5%) a sensitive control handle. Any small discrepancies observed between first/second/total order indices are fully resolved if confidence intervals are considered.

For clarity, confidence intervals are only presented for first and total order indices greater than 0.05. It is noted that some confidence intervals are large, however, the impact on control handle classification is small: all control handles classed as highly sensitive based on any of the key model outputs retain at least a sensitive classification if lower confidence bounds are used. No key control handles could have been overlooked due to uncertainty in the sensitivity indices, since no control handles currently classed as not sensitive have an upper confidence bound above the highly sensitive limit.

Total order sensitivity indices calculated based on EQI, OCI and total GHG emissions are presented in Figure 2, with the contribution of first and higher order effects shown.

Figure 2
In terms of their total order effects on GHG emissions, three control handles are classified as highly sensitive: $Q_w$, $KLa_1$ and $KLa_5$. $Q_w$ is also the greatest contributor to output variance in EQI and OCI and appropriate control of this control handle is, therefore, vital. The importance of wastage flow rate in terms of its effects on effluent quality and operational costs is already recognised, but by showing the sensitivity of GHG emissions to this control handle, this study highlights the necessity to consider all three performance indicators when selecting an appropriate value. EQI and OCI are also both either sensitive or highly sensitive to variation in $KLa_5$, suggesting that selection of an appropriate aeration intensity is key to the reduction of GHG emissions whilst maintaining an acceptable effluent quality and cost. This appears intuitive, since energy requirements for pumping and aeration contribute to both costs and emissions, yet it has been established in OAT sensitivity analysis that these control handles have a much greater effect on direct emissions than on those associated with energy consumption.

The aeration intensities $KLa_1$-4 all have a significant impact on GHG emissions but provide a greater contribution to output variance in emissions than in EQI, suggesting that a reduction in emissions with comparatively little impact on effluent quality should be achievable. Furthermore, reducing emissions without incurring additional costs may be possible since all
control handles to which GHG emissions are sensitive, except $Q_w$, have a higher total order sensitivity index based on GHG emissions than on OCI.

It is also found that interactions between control handles have a significant impact on both GHG emissions and EQI, accounting for 15% of variance in each output. As such, effective design of control strategies to reduce GHG emissions will need to consider the effects of using multiple control handles simultaneously and may require complex control algorithms.

Model predictive control of the DO setpoint and external carbon flow rate, for example, has been shown to enable reduced operating costs and improved effluent quality (Stare et al., 2007), although GHG emissions have not been considered. GSA results show that neither EQI, OCI nor GHG emissions are sensitive to adjustment of $Q_{intr}$, $Q_r$, $Q_{storage}$, $carb_2$ or $carb_3$ values, so optimisation of their values is of low priority and can be omitted to simplify the design problem.

Reduction of OCI – or correlation of OCI with chosen control handles values – ought to be straightforward since GSA reveals no significant interaction effects and shows variance to be predominantly (62%) attributable to variation in $Q_w$.

Second order indices are presented in Figure 3, in which the darkest colours denote control handle pairs to which the corresponding output is most sensitive. Control handle pairs
individually accounting for more than 5% are identified and, whilst no specific pairs are classified as sensitive based on more than one model output, all sensitive pairs (for any model output) are found to include $KLa_5$. This reinforces the importance of controlling $KLa_5$ if GHG emissions are to be reduced and an acceptable effluent quality maintained, and shows that interactions of $KLa_5$ with $Q_w$, $KLa_3$, $KLa_4$, $carb_1$, $carb_2$ and $carb_3$ must be taken into account. This appears reasonable since it is known, for example, that a low SRT, insufficient COD availability and low DO concentrations can lead to nitrite accumulation, which in turn can contribute to high $\text{N}_2\text{O}$ emissions (Kampschreur et al., 2009). It must be noted, however, that the impacts of $KLa_5$ adjustments and interactions may differ in practice due to model limitations; in this study, changes in $KLa_5$ have a large impact on conditions in the first reactor due to the use of a standard non-reactive clarifier model, but creation of anoxic conditions due to oxygen consumption can occur in a reactive clarifier (Guerrero et al., 2013), thereby preventing or reducing recirculation of oxygen.

Figure 3

For the EQI, no significant second order effects involving $Q_w$ are identified, showing that interaction effects visible in Figure 2 must be due to higher order effects. Selection of appropriate control handle values to improve effluent quality will be
challenging, therefore, since $Q_w$ is the greatest source of output variance and must interact with multiple control handles.

Analysis of the first and total order indices shows interaction effects to have negligible impact on the OCI, with only $Q_w$ involved in any identifiable interactions. This corresponds with the second order indices, in which no sensitive control handle pairs are found and the only interactions of note involve $Q_w$.

3.3 Key control handles for control strategy design

The results of OAT sensitivity analysis are used in conjunction with those of GSA to identify key control handles for the design of control strategies to reduce GHG emissions, since they give an indication of the likely direction of change whilst GSA explores the whole control handle space. To enable comparison, control handle rankings derived from the two analyses are summarized in Table 1. Results are also compared to identify important control handles which may be overlooked based on OAT sensitivity analysis alone. Control handles found to be most important in OAT sensitivity analysis are found to have significant effects in GSA, confirming that sensitive control handles have not been overlooked due to the reduced model stabilization and evaluation periods.

Table 1
OAT sensitivity analysis correctly identifies control handles classified as highly sensitive based on EQI and OCI in GSA as having the most significant effects. However, it does not enable identification of all control handles to which GHG emissions are highly sensitive due to the greater significance of interaction effects: $Q_w$ is ranked only 6th in OAT sensitivity analysis, but GSA shows it to be the second most important control handles, with its interactions contributing 7.7% of output variance. Simultaneous manipulation of $Q_w$ (to adjust SRT) and other control handles (such as aeration intensities) is an established approach to WWTP control, and the potential for improvements in effluent quality and operational costs has been demonstrated (e.g. Guerrero et al., 2012), but these results highlight the importance of considering interaction effects on GHG emissions also. No control handles which enable simultaneous improvement in EQI, OCI and GHG emissions through their first order effects alone were found, but trade-offs may be lessened or avoided when interactions are considered.

In this study, the impact of $Q_w$ on EQI is shown to be predominantly due to first order effects and OAT sensitivity analysis results suggest that adjustment is only likely to worsen effluent quality. It is also shown, however, that GHG emissions and OCI can both be reduced through the first order effects of $Q_w$. Given that interaction effects with $Q_w$ do contribute to variance in EQI, and significantly to variance in GHG
emissions, simultaneous improvements which are not revealed through OAT sensitivity analysis alone might be possible through appropriate control of \(Q_w\) and its interacting control handles.

All three outputs are sensitive or highly sensitive to adjustment of \(KLa5\). However, OAT sensitivity analysis shows that a decrease in \(KLa5\) corresponds with a significant reduction in GHG emissions and OCI but an increase in EQI, so adjustment to reduce emissions whilst maintaining acceptable effluent may not be straightforward. An increase in \(KLa5\) results in a small improvement in EQI but significantly worsens GHG emissions; this reinforces the necessity to consider the effects on GHG emissions when control is modified to improve effluent quality and supports previous recommendation that GHG emissions should be included as an evaluation criterion to provide a clearer picture of the overall suitability of WWTP control strategies (e.g. Flores-Alsina et al., 2014). GSA also shows \(KLa5\) to be involved in significant interaction effects, further complicating the design problem. In particular, the effects of interaction with \(Q_w\) on GHG emissions and interaction with \(KLa3\) on EQI should be considered.

GHG emissions are found to be highly sensitive to \(KLa1\) and sensitive to \(KLa2\), whilst effects of these control handles on EQI and OCI are insignificant. This might imply that adjustment of \(KLa1\) and \(KLa2\) could be used to reduce
emissions without incurring trade-offs; however, the base case value for both is zero and OAT sensitivity analysis shows only a significant increase in emissions resulting from change in $KLa1$ and $KLa2$. Therefore, although they have a significant impact on GHG emissions, there may be no benefits from altering the base case values as performance would only be worsened. Given the high sensitivity of $KLa1$, however, it is recommended that the effects of small alterations are investigated since these would be missed in OAT sensitivity analysis and may be beneficial.

Interaction effects involving $KLa3$ are shown to be particularly important, as GHG emissions would not be classified as sensitive to this control handle based on its first order effects alone. Given that neither EQI nor OCI are sensitive to $KLa3$ and OAT sensitivity analysis shows that adjustment to reduce emissions is possible, suitable control of aeration in the first aerobic reactor is likely to be key to the development of control strategies to reduce GHG emissions – although complex, given interactions mostly involve at least three control handles.

Appropriate control of $KLa4$ is also important, since it is classified as sensitive based on both EQI and GHG emissions. OAT sensitivity analysis reveals a trade-off: a reduction in GHG emissions due to individual adjustment of $KLa4$ corresponds to an increase in EQI, but because GSA shows the effects of interactions to involving $KLa4$ to be significant, it is
likely that the comparative magnitude of effects on each output differs across the range of feasible values and an optimum can be identified.

In GSA, carb1 is classified as sensitive based on OCI only and, as such, might be adjusted in an attempt to reduce cost with little impact on effluent quality or emissions. However, OAT sensitivity analysis shows that a decrease in OCI due to reduction of carb1 corresponds with an increase in GHG emissions. Therefore, if carb1 is lowered to reduce operational cost, it is vital that the impact on GHG emissions is considered and, if necessary, countered with other measures.

EQI, OCI and GHG emissions are not sensitive to Qintr, Qr, Qstorage, carb2 and carb3, suggesting that dynamic control of these control handles would be of little benefit. It is, therefore, recommended that optimisation of internal recirculation flow rate, return sludge flow rate, anoxic reactor carbon source addition rates (except in first reactor) and storage tank control is of low priority when developing new WWTP control strategies. It has been demonstrated that control strategy optimisation using this knowledge can enable substantial emission reductions whilst maintain an acceptable effluent quality and without increasing operational costs (Sweetapple et al., 2014).
3.4 Key emission sources for reduction of greenhouse gas emissions

Based on simulations undertaken for GSA, the base case value, mean and variance of emissions from different sources are detailed in Table 2. Total GHG emissions are decomposed into direct emissions of each gas and indirect emissions from each source, as well as those resulting from the wastewater line and sludge line. Wastewater line emissions include all direct emissions associated with the activated sludge reactors and indirect emissions resulting from effluent degradation and energy demand for reactor aeration and mixing, chemical consumption; sludge line emissions include those from biogas leakage, combustion and energy recovery, dewatering, energy for digester heating and mixing, and transport and offsite degradation of sludge. It is noted that variances reported are small in comparison with those resulting from model parameter uncertainties (Sweetapple et al., 2013), and future work should investigate the impact of modelling uncertainties on control strategy design.

Table 2

It is notable that, whilst direct CO$_2$ emissions are the greatest contributor to total GHG emissions (at 48%), their output variance is just 1.7% of that of direct N$_2$O emissions, which contribute only a comparatively small 24% of mean total GHG
emissions. Indirect emissions and direct CH$_4$ emissions contribute 28%, yet are found to have negligible variance. This shows that the source of emissions with the greatest scope for improvement does not necessarily correspond with the overall greatest source of emissions, and suggests that any reduction in GHG emissions resulting from modified control will be primarily due to a reduction in N$_2$O emissions. Control strategy development and optimisation should, therefore, focus on reduction of direct N$_2$O emissions, all of which result from wastewater processes (specifically, activated sludge), and it is important that N$_2$O emissions are carefully monitored to ensure that they are not unintentionally increased as a result of actions to improve effluent quality and/or reduce operational costs. Existing knowledge that a reduction in DO setpoint to reduce costs can result in an increased risk of N$_2$O production (Porro et al., 2014) supports this recommendation. A potential strategy for mitigating the risk whilst maintaining cost savings may include better control and distribution of the aeration (Porro et al., 2014).

Further sensitivity analysis is used to investigate key control handles affecting wastewater line and sludge line GHG emissions, and OAT sensitivity analysis results are presented in Figure 4.
In OAT sensitivity analysis it is shown that changes in total GHG emissions are predominantly due to variation in wastewater line emissions, with only $Q_w$ resulting in a change of emissions of more than 0.7% in the sludge line. In GSA also, variance in sludge line emissions is negligible in comparison with that of wastewater line emissions and is found to be primarily due to the first order effects of $Q_w$. The ranking of each control handle based on total order effects on wastewater line emissions is identical to that for total GHG emissions, but an additional sensitive control handle, $carb1$, is identified. The significance of first order effects of variation in $KLa3$ is also greater on wastewater line emissions than on total emissions, with the control handle classified now classified as sensitive based on its first order index.

OAT sensitivity analysis shows a decrease in $Q_w$, the only control handle to which sludge line emissions are sensitive, to correspond with a decrease in both sludge line and wastewater line emissions (and vice versa). WWTP modelling used during control strategy development for the reduction of GHG emissions could, therefore, justifiably omit sludge line emissions in order to reduce computational demand, since there is little potential for their reduction from improved control alone and any small change observed is likely to be a decrease if $Q_w$ is manipulated to aid reduction of wastewater line emissions.
4 CONCLUSIONS

This research has investigated the impact of adjusting 14 WWTP control handles, including flow rates, aeration rates and carbon source addition rates, to enable identification of key control handles and sensitive sources for the reduction of GHG emissions. Based on the results of OAT sensitivity analysis and Sobol’s method GSA, the following conclusions are drawn:

- It is vital to consider the effect on GHG emissions when developing control strategies to improve effluent quality and/or reduce cost as, in some instances, a small change in EQI and/or OCI resulting from the individual effects of adjusting a control handle corresponds with a significant change in GHG emissions, and trade-offs between objectives have been identified.

- Selection of suitable values for aeration intensity in the final tank and wastage flow rate in the activated sludge process is of key importance, and active control of these control handles may be beneficial, but it is essential that their impacts on GHG emissions are considered. Both have a significant individual impact on variance in all three model outputs, and EQI and GHG emissions are also sensitive to interaction effects involving the aeration intensity.
• Unless effluent quality and/or operational cost are to be sacrificed, it is necessary to consider the effects of adjusting two or more control handles together when developing control strategies to reduce GHG emissions, since no control handles enabling simultaneous improvement in EQI, OCI and GHG emissions through their individual effects alone were identified.

• Formation of N₂O in the activated sludge process is the source of GHG emissions with the greatest scope for improvement, and from which it is important that emissions are carefully monitored to ensure that they are not unintentionally increased as a result of actions to improve effluent quality and/or reduce operational costs.

• Dynamic control of internal recirculation and return sludge flow rates, reject water flow rate set point and carbon source addition in second and subsequent anoxic reactors would be of little benefit and it is recommended that optimisation of these control handles is of low priority since they were not classified as sensitive based on EQI, OCI or GHG emissions.

It is hoped that this knowledge will assist future development of WWTP control strategies to reduce GHG emissions whilst maintaining acceptable effluent quality and operating costs, and aid an efficient design and optimisation process.
ACKNOWLEDGEMENTS

Thanks are given for the Matlab/Simulink implementation of the BSM2 from the Department of Industrial Electrical Engineering and Automation, Lund University, Lund, Sweden, and for Dr Patrick Reed’s C++ code for implementation of Sobol’s sensitivity analysis. Christine Sweetapple gratefully acknowledges financial support provided by the University of Exeter in the form of a studentship.
REFERENCES


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FIGURE CAPTIONS

Fig. 1 – Percentage change in model outputs resulting from individual variation of control handles

Fig. 2 – First and total order indices calculated using Sobol’s method, based on EQI, OCI and total GHG emissions

Fig. 3 – Second order sensitivity indices calculated using Sobol’s method based on EQI and total GHG emissions

Fig. 4 – Change in wastewater line and sludge line GHG emissions resulting from variation of individual control handles, as a percentage of base case total GHG emissions
TABLE CAPTIONS

Table 1 – Ranking of control handles based on OAT sensitivity analysis and GSA

Table 2 – Characteristics of GHG emissions from key sources
Table 1 – Ranking of control handles based on OAT sensitivity analysis and GSA

<table>
<thead>
<tr>
<th>Control handle</th>
<th>Sensitivities based on EQI</th>
<th>Sensitivities based on OCI</th>
<th>Sensitivities based on total GHG emissions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>GSA sensitivity rank</td>
<td>OAT rank</td>
<td>GSA sensitivity rank</td>
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<tr>
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<td>First order</td>
<td>Total order</td>
<td>First order</td>
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<tr>
<td>carb5</td>
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<td>7</td>
<td>12</td>
</tr>
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</table>

Light grey shading denotes sensitive control handles, based on corresponding index
Dark grey shading denotes highly sensitive control handles, based on corresponding index
Table 2 – Characteristics of GHG emissions from key sources

<table>
<thead>
<tr>
<th></th>
<th>Direct emissions</th>
<th>Indirect emissions</th>
<th>Total wastewater line</th>
<th>Total sludge line</th>
<th>Total GHGs</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Direct CO₂</td>
<td>Direct CH₄</td>
<td>Direct N₂O</td>
<td>Net energy</td>
<td>Carbon source</td>
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<tr>
<td>Base case (kg CO₂e/m³)</td>
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<td>0.06</td>
<td>0.15</td>
<td>0.06</td>
<td>0.04</td>
</tr>
<tr>
<td>Mean (kg CO₂e/m³)</td>
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<td>0.06</td>
<td>0.24</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>Variance ((kg CO₂e/m³)²)</td>
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<td>0.00</td>
<td>0.03</td>
<td>0.00</td>
<td>0.00</td>
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