Supplementary Information

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

Christine Sweetapple[a*], Guangtao Fu[a], David Butler[a]

[a] Centre for Water Systems, College of Engineering, Mathematics and Physical Sciences, University of Exeter, North Park Road, Exeter, Devon EX4 4QF, United Kingdom

[*] Corresponding author. Tel.: +44 (0)1392 726652; E-mail: cgs204@ex.ac.uk

This supplement contains the following:

- **Figure S1**, a diagram of the wastewater treatment plant (WWTP) under study, with modeled sources of greenhouse gas (GHG) emissions indicated and control handles investigated shown.
- **Table S1**, details of control handles analyzed, including default values, maximum and minimum allowable values, and upper and lower limits used in sensitivity analysis.
- Equations for calculation of percentage change in model outputs for one-factor-at-a-time (OAT) sensitivity analysis.
- Information on the implementation of Sobol's method for global sensitivity analysis (GSA).
- A description and justification of the simulation strategies used for OAT and global sensitivity analyses.
- An explanation of the treatment of apparent discrepancies between sensitivity indices of different orders.
- **Figure S2**, graphical representation of first and total order sensitivity indices calculated based on wastewater line GHG emissions only

MATERIALS AND METHODS

1.1 Model description and available control handles

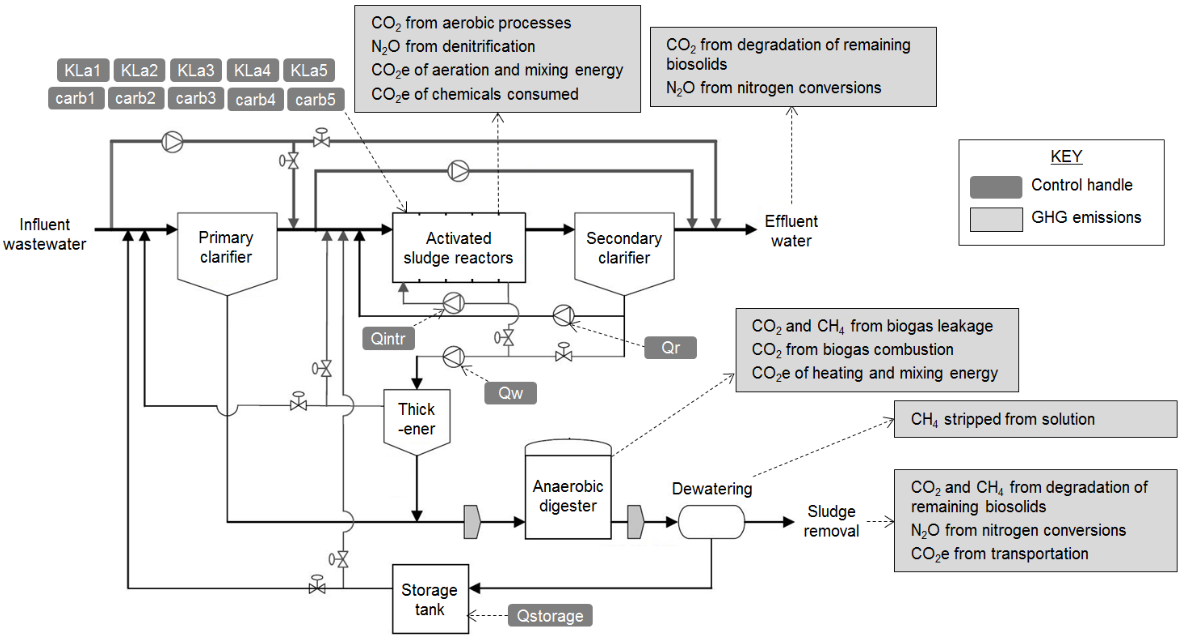

Figure S1. Schematic diagram of the WWTP, showing control handles studied and sources of modelled GHG emissions, adapted from Nopens *et al*. (2010)

Table S1. Feasible range of control handles and limits used for sensitivity analysis

Control handle	Notation	Values				
		Min.	Lower limit	Default	Upper limit	Max.
Internal recirculation flow rate (m^3/d)	Qintr	0	51,620	61,944	72,265	103,240
Return sludge flow rate (m^3/d)	Qr	0	16,518	20,648	24,778	41,296
Wastage flow rate (m^3/d)	Qw	0	93.5	300	506.5	2064.8
Reject water flow rate set point (m^3/d)	Qstorage	0	0	0	150	1500
Reactor 1 aeration intensity (d^{-1})	KLa1	0	0	0	24	240
Reactor 2 aeration intensity (d^{-1})	KLa2	0	0	0	24	240
Reactor 3 aeration intensity (d^{-1})	KLa3	0	96	120	144	240
Reactor 4 aeration intensity (d^{-1})	KLa4	0	96	120	144	240
Reactor 5 aeration intensity (d^{-1})	KLa5	0	36	60	84	240
Reactor 1 carbon source addition (m^3/d)	carb1	0	1.5	2	2.5	5
Reactor 2 carbon source addition (m^3/d)	carb2	0	0	0	0.5	5
Reactor 3 carbon source addition (m^3/d)	carb3	0	0	0	0.5	5
Reactor 4 carbon source addition (m^3/d)	carb4	0	0	0	0.5	5
Reactor 5 carbon source addition (m^3/d)	carb5	0	0	0	0.5	5

1.2 One-factor-at-a-time sensitivity analysis

Upper and lower bound outputs (***Y***) for control handle *i* are calculated using Eqs. 2 and 3 respectively, where *n* is the number of control handles, *x* is the control handle value and $x_{\sim i}$ denotes the value of all control handles except x_i.

$$\boldsymbol{Y}_{base} = f(x_{1\ldots n}) \tag{1}$$

$$\boldsymbol{Y}_{i,upper} = f(x_{i,max}, x_{\sim i}) \tag{2}$$

$$\boldsymbol{Y}_{i,lower} = f(x_{i,min}, x_{\sim i}) \tag{3}$$

Percentage change in model outputs with respect to the base case is then calculated as follows:

$$\boldsymbol{P}_{i,upper} = 100 \times \frac{\boldsymbol{Y}_{i,upper} - \boldsymbol{Y}_{base}}{\boldsymbol{Y}_{base}} \tag{4}$$

$$\boldsymbol{P}_{i,lower} = 100 \times \frac{\boldsymbol{Y}_{i,lower} - \boldsymbol{Y}_{base}}{\boldsymbol{Y}_{base}} \tag{5}$$

1.3 Global sensitivity analysis

To implement Sobol's method, quasi-Monte Carlo sampling with Sobol's sequence generator is first used to generate 2*n* random control handle samples (within the specified upper and lower bounds, and in this case using a uniform distribution). Control handles are then resampled to generate *n*(2*p*+2) sets, using Saltelli's extension to Sobol's method (Saltelli, 2002), and WWTP performance is evaluated using each set of control handle values in turn. First, second and total order sensitivity indices for each control handle or control handle pair are computed as detailed by Tang *et al*. (2007b) and corresponding 95% bootstrap confidence intervals are calculated.

GSA included all control handles detailed in Table S1, as all except two were found to have significant effects in OAT sensitivity analysis and the impact of interactions involving these is unknown. Analysis used a sample size of 2,000, which yielded 30,000 control handle sets for simulation when resampled. This value was selected on the basis of previous studies, in which it was found sufficient to achieve accurate and repeatable results with 18 and 21 parameters (Tang et al., 2007a; Fu et al., 2012). Bootstrapped confidence intervals were calculated using 1,000 resamples.

1.4 Simulation strategy

Simulations for assessment of control strategy performance in the BSM2 use 200 days of constant influent to allow the model to reach steady state, followed by 609 days of dynamic influent (of which the final 364 are for evaluation) (Jeppsson et al., 2007). This strategy is replicated for OAT sensitivity analysis of control handles in BSM2-e, with the model used in its open loop configuration (i.e. no sensors or controllers are implemented). Given the high computational demand of such simulations (due in part to the additional complexity of modelling dynamic GHG emissions) and the large number of model evaluations required for GSA, however, it is impractical to use the full stabilisation and evaluation period for further analysis.

In order to identify suitable reduced stabilisation and evaluation periods, additional OAT sensitivity analyses were undertaken and the effects of a range of different options on control handle rankings analysed. Maintaining a sufficiently long stabilisation period to reach dynamic ‘pseudo steady state’ was prioritised over the evaluation duration; given that the default SRT of the anaerobic digester is 19 days, the model may not reach quasi steady-state with a reduced stabilisation period, but the stabilisation must be sufficient to allow the relative significance of the effects of each control handle to be assessed. Based on the OAT sensitivity analysis results, it was decided to use a 200 day steady-state simulation (using the BSM2 constant influent data but with temperature adjusted to equal that at the start of the dynamic influent) followed by a 56 day dynamic simulation (using days 294-350 of the BSM2 dynamic influent data), with the final 14 days used for performance evaluation. Although not fully replicating model outputs from the full length simulation, this reduced period was found to be suitable for assessing the relative importance of each control handle: it allowed correct identification of the most sensitive control handles and resulted in a mean absolute change in OAT sensitivity analysis rank of just 0.71 for all control handles across the three key outputs when compared with the results of analysis using the full, 609 day dynamic simulation period.

RESULTS

1.5 Sobol's method sensitivity indices

Some slightly negative indices are observed for all performance indicators; these are assumed to equal zero, as in previous studies (Tang et al., 2007a; Tang et al., 2007b), since it is known that truncation of Monte Carlo approximations used to calculate integrals in Sobol's method can lead to small numerical errors (Tang et al., 2007b). This also accounts for instances in which the total order sensitivity index is less than the sum of the first and second order indices (which are observed primarily for not sensitive control handles), and the fact that first order indices based on OCI sum to 1.03.

1.6 Key emission sources for reduction of greenhouse gas emissions

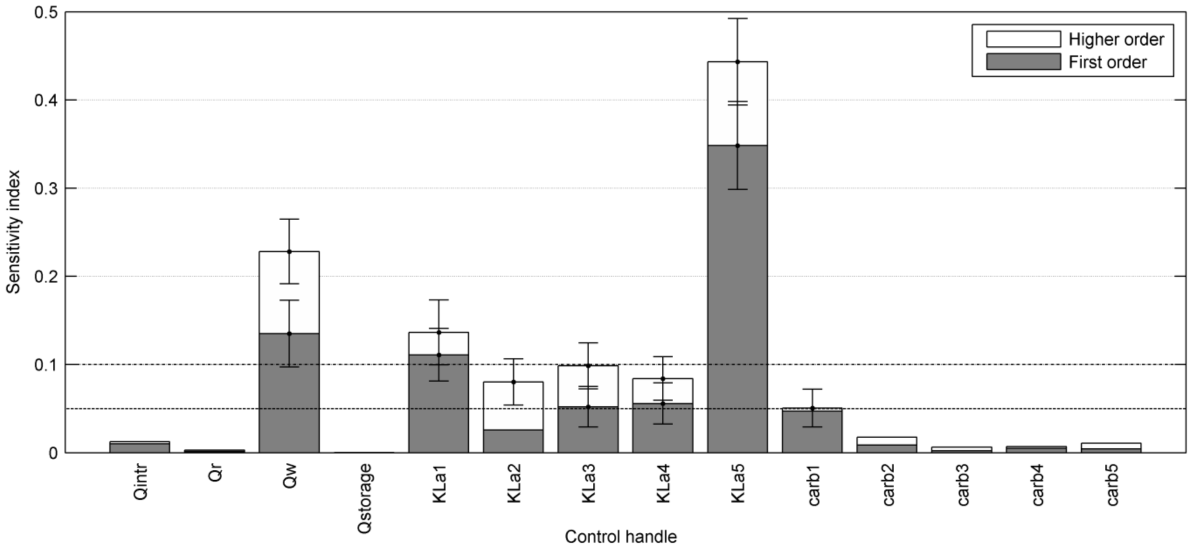

Figure S2. First and total order sensitivity indices based on wastewater line GHG emissions

REFERENCES

Fu, G. T., Kapelan, Z. & Reed, P. 2012. Reducing the Complexity of Multiobjective Water Distribution System Optimization through Global Sensitivity Analysis. *Journal of Water Resources Planning and Management-Asce,* 138(3)**,** 196-207.

Jeppsson, U., Pons, M. N., Nopens, I., Alex, J., Copp, J. B., Gernaey, K. V., Rosen, C., Steyer, J. P. & Vanrolleghem, P. A. 2007. Benchmark simulation model no 2: general protocol and exploratory case studies. *Water Science and Technology,* 56(8)**,** 67-78.

Nopens, I., Benedetti, L., Jeppsson, U., Pons, M. N., Alex, J., Copp, J. B., Gernaey, K. V., Rosen, C., Steyer, J. P. & Vanrolleghem, P. A. 2010. Benchmark Simulation Model No 2: finalisation of plant layout and default control strategy. *Water Science and Technology,* 62(9)**,** 1967-1974.

Saltelli, A. 2002. Making best use of model evaluations to compute sensitivity indices. *Computer Physics Communications,* 145(2)**,** 280-297.

Tang, Y., Reed, P., van Werkhoven, K. & Wagener, T. 2007a. Advancing the identification and evaluation of distributed rainfall-runoff models using global sensitivity analysis. *Water Resources Research,* 43(6).

Tang, Y., Reed, P., Wagener, T. & van Werkhoven, K. 2007b. Comparing sensitivity analysis methods to advance lumped watershed model identification and evaluation. *Hydrology and Earth System Sciences,* 11(2)**,** 793-817.