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Identifying key sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment

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ABSTRACT

This study investigates sources of uncertainty in the modelling of greenhouse gas emissions from wastewater treatment, through the use of local and global sensitivity analysis tools, and contributes to an in-depth understanding of wastewater treatment modelling by revealing critical parameters and parameter interactions. One-factor-at-a-time sensitivity analysis is used to screen model parameters and identify those with significant individual effects on three performance indicators: total greenhouse gas emissions, effluent quality and operational cost. Sobol's method enables identification of parameters with significant higher order effects and of particular parameter pairs to which model outputs are sensitive. Use of a variance-based global sensitivity analysis tool to investigate parameter interactions enables identification of important parameters not revealed in one-factor-at-a-time sensitivity analysis. These interaction effects have not been considered in previous studies and thus provide a better understanding wastewater treatment plant model characterisation. It was found that uncertainty in modelled nitrous oxide emissions is the primary contributor to uncertainty in total greenhouse gas emissions, due largely to the interaction effects of three nitrogen conversion modelling parameters. The higher order effects of these parameters are also shown to be a key source of uncertainty in effluent quality.

1. Introduction

Wastewater treatment can result in direct emissions of greenhouse gases (GHGs) such as carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O), as well as indirect emissions resulting from energy generation, chemical manufacture and sludge disposal, amongst other sources. Reduction of GHG emissions is a topic of global interest, and it is recognised that appropriate design and operation of wastewater treatment processes can play a significant role in mitigating the effects of global warming (Gori et al., 2011).

Models used to estimate the magnitude of GHG emissions from wastewater treatment plants (WWTPs) for inventories typically utilise empirical emission factors (e.g. IPCC, 2006b), based on the volume of wastewater treated, influent concentrations, effluent concentrations or the mass of wastewater components removed. These emission factors, however, have a high degree of variability and uncertainty (Corominas et al., 2012): for example, N_2O emissions in the range 0–90% of the nitrogen-load were reported by Kampschreur et al. (2009). As such, there has been increasing interest in the use of comprehensive process models and mechanistic models to

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estimate dynamic GHG emissions. Resulting from this, it has been highlighted that significant variability can occur in GHG emissions from WWTPs with different designs (Shahabadi et al., 2009) and operating under different conditions (Flores-Alsina et al., 2011).

As wastewater utilities face the challenge of simultaneously reducing GHG emissions and improving treatment standards due to increasing regulatory pressures, the importance of including GHG emissions in addition to effluent quality and operational costs when evaluating design alternatives is clear. It has been shown that use of automatic control can reduce GHG emissions (Corominas et al., 2010), but models used are typically of hypothetical WWTPs and their results are not always validated with real data (e.g. Hiatt and Grady, 2008; Guo et al., 2012). As such, results are likely to be subject to a high degree of uncertainty; and careful calibration is therefore essential if applying the models and estimation methodologies to a real WWTP for plant design or control strategy development to reduce GHG emissions. Identification of the most significant sources of uncertainty could aid efficient calibration of models and reduce the complexity of future uncertainty analyses, yet there has been little research into the magnitude of uncertainty in GHG emission estimates resulting from uncertainty in model parameters and emission factors.

Sensitivity analysis is a useful tool for identification of the key parameters controlling model outputs (Tang et al., 2007a). However, whilst sensitivity analyses of dynamic WWTP models have previously been undertaken to investigate the effects of uncertainty in model parameters (e.g. Pons et al., 2008; Flores-Alsina et al., 2009; Ramin et al., 2012), design and operational parameters (Benedetti et al., 2008; Pons et al., 2008) and influent characteristics (Pons et al., 2008), no detailed analyses for identification of key parameters affecting GHG emissions have been carried out. Gori et al. (2011) completed a sensitivity analysis to investigate the effects of varying the pCOD/VSS ratio on the rate of GHG emissions from different sources, but no other model parameters were considered. Global sensitivity analyses (GSAs) of the Benchmark Simulation Model No. 1 (BSM1) (Sin et al., 2011) and the Benchmark Simulation Model No. 2 (BSM2) (Benedetti et al., 2008), based on Monte Carlo experiments and linear regression, enabled the identification of individual parameters with significant effects on effluent quality and operational cost, but did not consider GHG emissions. However, interactions were not investigated and output uncertainty was attributed to individual parameters only.

The aim of this research is to identify individual parameters and parameter interactions which contribute significantly to uncertainty in modelled GHG emissions from wastewater treatment, as well as the more widely used performance indicators of effluent quality and operational cost. Investigation of the relative contributions of specific parameter interactions to output uncertainty represents an advance in WWTP modelling, as previous analyses have not enabled identification of significant interactions. Sensitivity analysis of a revised BSM2, with pre-defined layout, operating conditions and influent characteristics, is carried out using the one-factor-at-a-time (OAT) method, to identify significant individual (first order) effects and inform the selection of parameters for inclusion in further analysis. GSA is then carried out using a variance-based method – Sobol's method (Saltelli, 2002) – to investigate higher order effects (interactions). This tool has not, as of yet, been extensively used in wastewater treatment, but previous applications have revealed situations and modelling scenarios in which calibration is likely to be most challenging due to the greater presence of parameter interactions (Massmann and Holzmann, 2012) and improved the efficiency of multi-objective optimisation problems by identifying important decision variable interactions (Fu et al., 2012). The results enable identification of: a) parameters that have negligible impact on uncertainty in key model outputs and can, therefore, be excluded from future uncertainty analyses; and b) parameters which contribute significantly to variance in any key model output, due to first or higher order effects, and so need to be accurately defined for model calibration and application.

2. Materials and methods

2.1. *Model description*

2.1.1. *Model structure*

The WWTP model used for parameter sensitivity analysis, which will be referred to as BSM2-e, is based on the Benchmark Simulation Model No. 2: BSM2 (Jeppsson et al., 2007), with modifications (outlined in Section 2.1.2) made to enable dynamic modelling of the emissions shown in Fig. 1. The plant layout and modelling of pre-treatment and sludge treatment processes are unaltered from those of BSM2 (as detailed by Jeppsson et al. (2007) and Nopens et al. (2010)), but adjustments have been made to the activated sludge model to enable calculation of N_2O emissions. A complete description of all equations added and modifications made to the BSM2 is provided as Supplementary information.

2.1.2. *Greenhouse gas emission modelling methodologies*

GHG emissions are modelled using previously published estimation methodologies, which are implemented in BSM2. Sources of GHG production and direct emissions from the modelled processing units include:

- Aerobic substrate utilisation (CO_2), biomass decay (CO_2) and denitrification (CO_2 and N_2O) in activated sludge reactors

In BSM2, the reduction of nitrate to nitrogen is modelled as a one-step process and dynamic production of N_2O (an intermediate product) cannot be determined. Modifications have therefore been made to include four-step denitrification as detailed by Samie et al. (2011). Stripping of N_2O from solution is then modelled using Henry's law. CO_2 emissions resulting from nutrient removal are calculated using emission factors derived from the stoichiometric relationships for denitrification with and without an external carbon source (Shahabadi et al., 2010).

Calculation of CO_2 emissions from substrate utilisation and biomass decay is based upon the method detailed by Monteith et al. (2005), with the suspended solids mass balance equation adapted for non-steady state conditions. Required