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Sensitivity and uncertainty analysis of a plant-wide model for carbon and energy footprint of wastewater treatment plants

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Abstract: This paper presents the sensitivity and uncertainty analysis of a mathematical model for Greenhouse gas (GHG) and energy consumption assessment from wastewater treatment plants (WWTPs). The model is able to simultaneously describe the main biological and physical-chemical processes in a WWTP. Specifically, the mathematical model includes the main processes of the water and sludge lines influencing the methane (CH_4), nitrous oxide (N_2O), and carbon dioxide (CO_2) emissions. Further, the process energy demand and the energy recovery are also taken into account. The main objective of this paper is to analyze the key factors and sources of uncertainty influencing GHG emissions from WWTP at a plant-wide scale. The results show that influent fractionation has an important role on direct and indirect GHGs production and emission. Moreover, model factors related to the aerobic biomass growth show a relevant influence on GHGs in terms of power requirements. Thus, a good WWTP design and management aimed at limiting the GHG emission should carefully take into account the aeration system model to reduce GHG emission associated with electrical power demand. Also, the N_2O emission associated with the effluent has the highest relative uncertainty bandwidth (1.7), suggesting one more need for a mechanistic model for N_2O production in biological treatment.

Keywords: Modelling, energy demand, green house gas emission, uncertainty.

1. INTRODUCTION

The interest for greenhouse gas (GHG) emissions from wastewater treatment plants (WWTPs) has considerably increased in the recent past (Monteith et al, 2005; Kampschreur et al., 2009; Flores-Alsina et al., 2011; Corominas et al., 2012; Law et al., 2012). WWTPs involve three different sources of GHGs emission: direct, indirect internal and indirect external (GRP, 2008). These three sources belong to the scopes established by the World Resources Institute (WRI) and the World Business Council for Sustainable Development (WBCSD) in the GHG Protocol Standard to classify emissions (scope 1, scope 2, and scope 3). The three scopes provide a comprehensive framework to account, manage and reduce direct and indirect emissions. Direct emissions of WWTPs are mainly related to the biological processes (emission of carbon dioxide-CO_2 from biomass respiration; biogas fugitive emissions from digesters and gas lines); indirect internal emissions are associated with the consumption of purchased or acquired electric or thermal energy; finally indirect external emissions are related to all that sources not directly controlled inside the WWTP (e.g., sludge disposal, production of chemicals that are used in the plant). The main GHG emitted from a WWTP are CO_2, methane (CH_4) and nitrous oxide (N_2O). The fraction of short-lived carbon in the wastewater is not of concern for CO_2 emission, while attention must be given to long-lived carbon and the other GHGs (Law et al, 2013). Among the GHGs emitted from WWTPs, N_2O merits to be investigated and reduced due to its high global warming potential (GWP) that is about 298 times bigger than for CO_2 (IPCC, 2006). Therefore, even low amounts of N_2O emission are undesired and raise concern. Regardless of

the carbon origin, a quantification of GHGs is necessary to improve our understanding of carbon flows within treatment and the sustainability of WWTPs. Furthermore, the estimation of GHGs should be considered during the design, operation and optimisation of WWTPs (Flores-Alsina et al., 2011). With this regard several attempts to better understand the GHG production processes (Joss et al., 2009; Foley et al., 2010; Daelman et al., 2012), to quantify and measure GHG emissions (GWRC, 2011) and to predict and control their production (Corominas et al., 2012; Flores-Alsina et al., 2011; Ni et al., 2013a-b) have been performed over the years. Literature shows that knowledge on the dynamics and magnitude of N_2O formation/emissions is still poor and that further investigations have to be performed (Kampschreur et al., 2009). With regards to the GHG quantification and measuring techniques, literature shows a wide range of measured GHG emissions (mainly N_2O) (GWRC, 2011; Daelman et al., 2012). This wide range reveals the need for improving our understanding of process dynamics as well as the measurement techniques and tools for GHG quantification. Plant-wide mathematical models can help in understanding the effect of operational parameters on GHG emission and can be used to develop strategies aimed at reducing GHG emissions and improving environmental protection. In fact, mathematical models allow to identify the key processes and the operational conditions that merit to be further investigated or modified in order to reduce GHG emissions. Different types of mathematical models (i.e., empirical, mechanistic, or simple comprehensive process models) are available for estimating GHG emissions (e.g., Monteith et al., 2005; Hiatt and Grady, 2008; Rosso and Stenstrom, 2008; Foley et al, 2010; Gori et al., 2010; Flores-Alsina et al., 2011; Gori et al., 2011; Ni et al., 2011). All these models have provided a valuable contribution to better understand how to reduce the GHG emissions from WWTPs. Further, as recently discussed by Flores-Alsina et al. (2013), a plant-wide modelling approach that includes GHG emissions as state variables enhances the overall sustainability view of the plant control/operational strategies. Indeed, by using a plant-wide approach modeller can include all the possible sources of GHG emissions (scopes 1-3) and discriminate the GHG contribution of each individual unit process. However, despite the useful insights derived by mathematical models of GHG emissions from WWTPs, the results are likely to be subjected to a high degree of uncertainty (Sweetapple et al., 2013). The GHG model predictions are strictly influenced by several factors: the knowledge of the modelled processes; the quality of the measured data used for calibrating the model parameters; the model structure. Thus, the uncertainty assessment in GHG emissions modelling can be useful in order to improve the model prediction. In this context both sensitivity and uncertainty analyses can be useful tools for identifying the key sources that control model outputs (Tang et al., 2007). Despite their potential, few uncertainty and sensitivity analyses to estimate carbon and energy footprint of WWTPs have been presented in literature.
In this study the key sources of uncertainty in GHG emission and energy requirement modelling have been identified. A plant-wide model for carbon and energy footprint of WWTPs previously developed has been used and the Extended-FAST method has been employed for the sensitivity analysis.

2. MATERIALS AND METHODS

2.1 Plant and mathematical model description

The model used for the analysis employed in this study was developed for modelling carbon and energy footprint of a conventional activated sludge WWTP based on a modified Ludzak-Ettinger process for denitrification, with primary sedimentation, anaerobic stabilization of the sludge and energy recovery from biogas. The total $CO_{2,eq}$ emission (kg_{CO2eq}/d) is calculated as the sum of: direct CO_2 emission from biological processes ($m_{CO2,ASP} + m_{CO2,AD}$); direct CO_2 emission from biogas combustion ($m_{CH4,comb}$); indirect CO_2 emission from off-site power generation ($m_{CO2eq,PG}$); $CO_{2,eq}$ offset from biogas energy recovery ($m_{CO2eq,offset}$); $CO_{2,eq}$ emission due to CH_4 fugitive emission ($mCO_{2eq,fugitive}$):

$$m_{CO_2eq} = m_{CO_2,ASP} + m_{CO_2,AD} + m_{CO_2,CH_4comb} + m_{CO_2eq,PG} - m_{CO_2eq,offset} + m_{CO_2,fugitive} \quad [1]$$

For the energy demand (e_D) the model estimates the contributions from primary sedimentation ($e_{D,PS}$), activated sludge process aeration ($e_{D,ASP}$), secondary sedimentation ($e_{D,SS}$), anaerobic digestion ($e_{D,AD}$), and other equipment ($e_{D,O}$):

$$e_D = e_{D,PS} + e_{D,ASP} + e_{D,SS} + e_{D,AD} + e_{D,O} \quad [2]$$

while for the energy recovery (e_R) is calculated from the biogas production m_{BG} (kg/d) times the efficiency of the energy unit recovery η_{ER} (-) and the caloric value of the biogas h_{BG} (kJ/kg_{BG}):

$$e_R = \eta_{ER} h_{BG} m_{BG} \quad [3]$$

For a detailed description of the model and case study refer to literature (Gori et al., 2011; 2013).

2.2 Sensitivity analysis method

Sensitivity analysis has been performed by using the Extended-FAST method. This method was proposed by Saltelli et al. (1999). Compared to the classical FAST method, Extended-FAST uses a new expression to deduce the optimal sampling curve in order to obtain a more flexible sampling scheme. This method belongs to the global sensitivity analysis methods and is based on the variance decomposition theorem. The Extended-FAST method provides two sensitivity indices for each i-th model factor: the first-order effect index (S_i) and the total-effect index (S_{Ti}). Si quantifies the contribution of the i-th model factor to the variance of the model output [Var(Y)] without considering the interaction among the model factors; it is expressed as:

$$S_i = \frac{Var_{xi}\left(E_{x_{-i}}\left(Y|x_i\right)\right)}{Var\left(Y\right)} \quad [4]$$

where E is the expectancy operator and Var is the variance. The subscripts indicate that the operation is either applied ''over the i-th factor'' Xi, or ''over all model factors except the i-th model factor'' X-i (Saltelli et al., 2004).
S_{Ti} is expressed as:

$$S_{T_i} = 1 - \frac{Var_{x_{-i}}\left(E_{x_i}\left(Y|x_{-i}\right)\right)}{Var\left(Y\right)} \quad [5]$$

The difference between S_{Ti} and S_i represents the interaction among the model factors. The Extended-FAST method requires nxNR simulations, where n is the number of factors and NR is the number of runs per model factor (NR = 500 – 1000 according to Saltelli et al., 2005).

2.3 Uncertainty analysis

The uncertainty analysis has been performed by running Monte Carlo simulations; results of the uncertainty analysis for each variable have been interpreted by analysing the cumulative distribution function (CDF). Moreover, the comparison of the uncertainty analysis results among the model outputs taken into account has been performed by comparing the value of the relative uncertainty bandwidth. This latter has been computed by dividing the width between the 5th and 95th percentiles to the 50th percentile.

2.4 Simulation conditions and numerical settings

Sensitivity analysis has been performed by considering 26 model factors (influent fractionation parameters, kinetic parameters, conversion factors, CH_4 specific energy and emission factors) and 10 model outputs. For a detailed description of the symbol and variation range of each factor the reader is referred to Gori et al. (2011) and Mannina et al. (2011). Due to the lack of knowledge about the distribution of the model factors, a uniform prior distribution was considered for each factor. The widest variation range found in literature has been used for each model factor. The Extended-FAST method was applied using the sensitivity package developed by Pujol (2007) in the R environment (R Development Core Team, 2007). To classify important, non-influential and interacting factors, the thresholds of the sensitivity measures were selected. Factors with Si value greater than 0.02, at least for one model output, were classified as important. Interacting model factors were selected using the normalised index value (S_{Ni}), which corresponds to the ratio between the interaction of the i-th model factor related to one model output and the maximum value among the interactions for that model output (Cosenza et al., 2013). Factors with S_{Ni} greater than 0.5 for at least one model output were considered to be interacting. Model factors with S_{Ni} and S_i values lower than 0.5 and 0.02, respectively, were considered to be non-influential. The uncertainty analysis was performed by all the model factors. The same number of simulations used during the Extended-FAST application has been used to perform the uncertainty analysis.

3. RESULTS AND DISCUSSION

3.1 Sensitivity analysis

The Extended-FAST method has been applied by running 26,000 model simulations and generating a model factor matrix with NR=1000. The sum of Si explains more than 90% of the total variance for all model outputs except for the power requirements. These results indicate that the model is linear and additive. This statement is also confirmed by the value of the sum of S_{Ti}, which is always close to 1 except for the power requirements. Indeed, results related to the power requirements show that for this model output quite a high degree of interaction among factors takes place (sum of S_{Ti} = 4.761). Results show that except for power requirements and η_{CODPS}, all important model factors are interacting with each other. Hence, the high degree of linearity flattens the selection of interacting factors for the great part of the model outputs analysed.
For sake of conciseness only the results related to CO_{2_resp}, CH_{4_comb}, $CH_{4\_dewatering}$ and power requirements (shown in Fig. 1) will be discussed in details. By analysing Fig. 1 one may observe that four factors have significant impact for CO_{2_resp} (Fig. 1a). Specifically k_d, $nbsCOD_{IN}$, $pbCOD_{IN}$ and $npbCOD_{IN}$ have an S_i value higher than 0.02 for CO_{2_resp}. Among these four factors, three ($nbsCOD_{IN}$, $pbCOD_{IN}$ and $npbCOD_{IN}$) are related to the influent wastewater fractionation and one (k_d) is related to the heterotrophic biomass kinetics. The effect of influent fractionation is certainly the most interesting from a process' point of view. In fact, the influent fractionation factors influence the bCOD availability to biomass growth and consequently the CO_{2_resp} value. For example, the higher the $nbsCOD_{IN}$ fraction and the lower the availability of substrate to be degraded during the biomass metabolism. Hence, CO_{2_resp} is reduced as a result of the conservative nature of $nbsCOD_{IN}$. Factor k_d represents the specific decay rate of heterotrophic biomass and significantly influence CO_{2_resp} because regulates the endogenous decay of heterotrophic biomass. For CH_{4_comb} (Fig. 1b), results show that k_d, pCOD/VSS, $pbCOD_{IN}$, $npbCOD_{IN}$, $pbCOD_{PI}$ and $npbCOD_{PI}$ appear to have a significant impact on the basis of S_i (all of these, except $npbCOD_{PI}$, are also interacting).

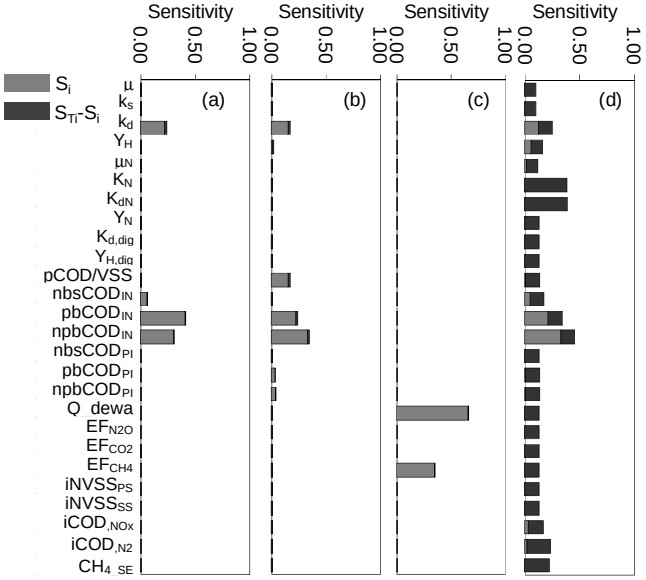

Fig. 1. Sensitivity (S_i) and interaction (S_{Ti} - S_i) of all factors for CO_{2_resp} (a), CH_{4_comb} (b), $CH_{4\_dewatering}$ (c) and Power requirements (d).

Among these factors the most relevant for process diagnostics are pCOD/VSS, $pbCOD_{IN}$ and $npbCOD_{IN}$. The fraction of pbCOD or npbCOD strongly influence the amount of CH_4 produced during anaerobic digestion due to the different nature of the bCOD removed in the primary settler. In fact, higher particulate in the influent wastewater entails higher bCOD removal in the primary settler, whose sludge is typically higher in COD per unit VSS mass removed than secondary sludge (Gori et al., 2011). This circumstance leads to an increase of the CH_4 production in the anaerobic tank and consequently of the equivalent CO_2 emitted during the combustion of CH_4 (Gori et al, 2013). Two factors have significant impact on $CH_{4\_dewatering}$ (Fig. 1c), namely $Q_{\_dewa}$ and EF_{CH4}. Indeed, these factors represent, respectively, the percentage of flow (respect to the influent wastewater flow) that reaches to the dewatering section and the emission factor of CH_4 from the dewatering.

For the power requirements model output, five factors resulted to be important in terms of S_i: k_d, Y_H, $nbsCOD_{IN}$, $pbCOD_{IN}$ and $npbCOD_{IN}$. Among these factors the first two are directly related to the kinetics of the heterotrophic biomass growth. Thus, since the WWTP energy demand is mainly due to the activated sludge processes (Rosso and Stenstrom, 2005; WEF, 2009), the influence of k_d and Y_H on the power requirements model output is associated with their influence on regulating the heterotrophic active biomass in the aerobic tank and consequently on the aeration energy requirements. A comment can be made on the relationship between temperature, biokinetics, and carbon footprint: as global temperature rise, the wastewater temperature rises, hence the value of k_d. Since k_d has a non-linear response with temperature increase (it increases by nearly an order of magnitude between 10 and 30 ^{0}C), and since in the same temperature range the bacterial efficiency in removing bCOD from the influent changes by a small adjustment, the consequence is that increasing temperatures should result in CO_2 emission from endogenous respiration (driven by k_d) that are higher in proportion than the CO_2 emission from aerobic respiration, in essence a positive feedback mechanism for CO_2 emission. The influence of $nbsCOD_{IN}$, $pbCOD_{IN}$ and $npbCOD_{IN}$ is mainly due to the ability of these factors to regulate the availability of soluble COD required for the biological processes. For example, as the fraction of sCOD decreases the oxygen required for the aerobic processes decreases thus influencing the power requirements of the aeration process and of the entire WWTP. High interaction among factors has been found for the power requirements model output. The high interaction is mainly due to the complexity of the model in terms of power requirements. The total power requirements are computed by summing the single processes' power requirements. It is important to underline that among the interacting factors, the factors having the highest contribution to the total model variance are k_N and k_{dN}. These two model factors are related to the kinetics of the autotrophic biomass. In fact, autotrophic biomass growth influences the aeration requirement inside the aerobic tank.

3.2 Uncertainty analysis

The uncertainty analysis was performed by considering all the 26 model factors. This analysis was applied by running the same number of simulations used for the Extended-FAST application. In Fig. 2, the cumulative distribution functions (CDFs) for CO_{2_resp}, CH_{4_comb}, $CH_{4\_dewatering}$ and power requirements are shown with the indication of the 5th and 95th percentiles. From a visual inspection of Fig. 2 one may observe that the width of the uncertainty bands, which is the difference between 95th and 5th percentiles, changes with the model output. This is mainly due to the fact that some of the model outputs entail a different level of complexity in terms of involved phenomena. Specifically, the uncertainty bands width of CO_{2_resp} (793 kg CO_2 m^{-3}) and CH_{4_comb} (597 kg CO_{2eq} m^{-3}) are higher than $CH_{4\_dewatering}$ (5 kg CO_{2eq} m^{-3}) and power requirements (229 kg CO_{2eq} m^{-3}). However, the width of the uncertainty band can be influenced by the order of magnitude of the considered model output.

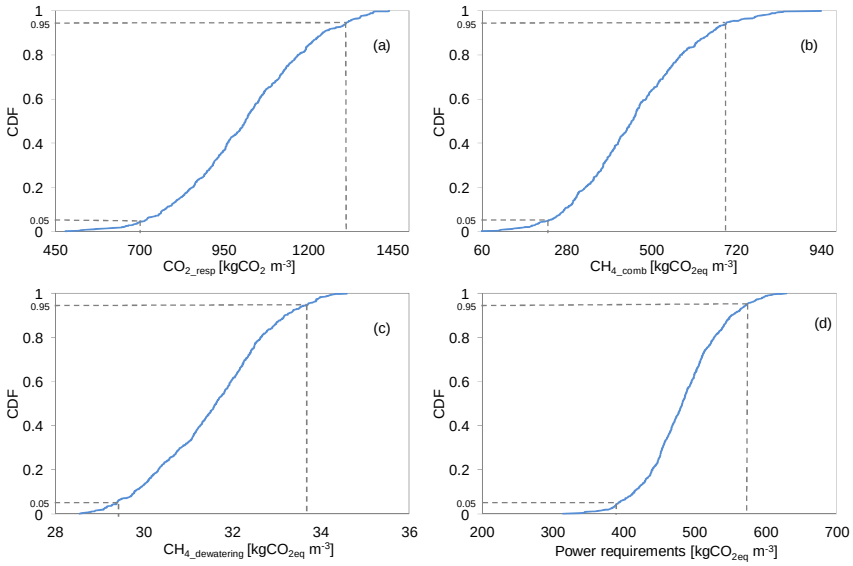

Figure 2. CDF of CO_{2_resp} (a), CH_{4_comb} (b), $CH_{4\_dewatering}$ (c) and Power requirements (d).

Thus, in order to provide a quantitative assessment of the model uncertainty and to make comparable the results among the model outputs, the relative uncertainty band width for each model output has been computed.
In Fig. 3 the relative uncertainty band widths for each model output are reported. By analysing Fig. 3 one may observe that the highest uncertainty is related to the N_2O emission due to the treated effluent (the relative uncertainty bandwidth is equal to 1.63).This fact may be due to the value of the EF_{N2O} used to quantify $N_2O_{effluent}$. This latter EF is based on the IPCC (2006) recommendation. However, as reported in literature, the EFs suggested by IPCC are highly uncertain due to the wide range of measured values used for EF definition. Within this context, the N_2O emission quantification could be improved by including the processes occurring in the receiving water body. In fact, if bCOD or nutrients are not removed inside a process they undergo inexorable (albeit slow) biodegradation in the receiving environment, which is the carbon footprint of no treatment (Rosso and Stenstrom, 2008).
From Fig. 3 one can also observe that a high and comparable uncertainty degree was found for CO_{2_comb}, CH_{4_comb}, $CH_{4\_fugitive}$ and Energy recovery (the relative uncertainty bandwidth is around 1.2 for the four model outputs).
The high uncertainty for these latter model outputs can be attributed to the complexity of the processes and consequently of the algorithms that describe their dynamics. These algorithms involve several model factors such as the influent COD fractionation, pCOD/VSS and the COD fractionation factors related to the primary effluent. Future studies, based on measured data, should be performed in order to clearly split the role of the uncertainty of each factor involved in the CO_{2_comb}, CH_{4_comb}, $CH_{4\_fugitive}$ and Energy recovery model outputs.

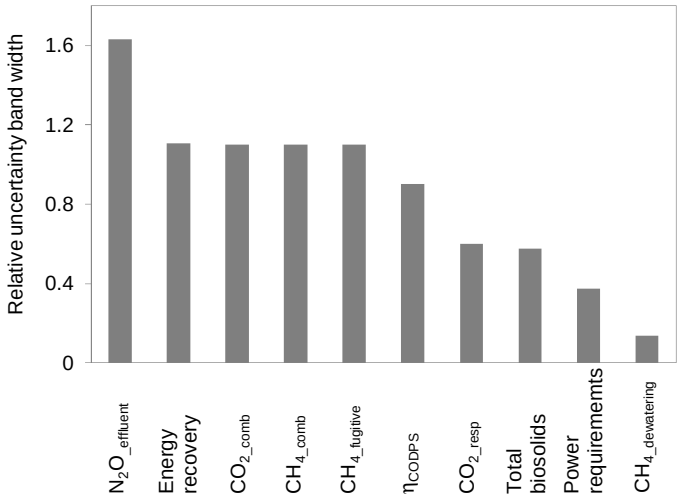

Figure 3. Relative uncertainty bandwidth for each model output.

4. CONCLUSIONS

The key findings of this study are summarised as follows:

- ✓ The sensitivity analysis reveals that model factors related to the influent wastewater and primary effluent COD fractionation exhibit a significant impact on all the analysed model outputs.
- ✓ The role of factor pCOD/VSS was found to be relevant especially in terms of interaction with the other factors; pCOD/VSS influences both the biomass activity inside the activated sludge system than the CH_4 production (and consequently CH_{4_comb}) during the anaerobic digestion.
- ✓ The uncertainty analysis reveals that $N_2O_{effluent}$ has the highest uncertainty in terms of relative uncertainty band (1.63) thus suggesting the need for improving the EF used for the $N_2O_{\_effluent}$ quantification.
- ✓ Results of the uncertainty analysis show that the uncertainty of model prediction increases after fixing non-influential factors. These results could be due to the default value of the non-influential factors. A calibration of the non-influential factors could be also be required in order to reduce uncertainty.

Overall, this study allowed gaining insights about the key model factors influencing the direct and indirect GHG emissions, on a plant-wide scale. In the future, efforts should be made in setting up an accurate data base to use for model calibration to reduce model uncertainty.

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