

Development of a Nonlinear Model Predictive Controller of Flexible Structure for Greenhouse Gas Emissions Minimisation in Pulp and Paper Wastewater Treatment Processes

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It is a well-established fact that activated sludge Wastewater Treatment Plants (WWTP) are placed among the most significant contributors of Greenhouse Gas (GHG) emissions. The task of intelligent emission control of such plants is a great challenge, mainly due to the highly nonlinear dynamics and associated uncertainty of its constituent bioprocesses. The need for more efficient and environmentally conscious control is ever increasing, due to the upsurge of industrial and urban water usage. In the current work, a nonlinear Model Predictive Control (MPC) scheme that considers an activated sludge model is developed for pulp and paper industry. The nonlinear MPC employs a flexible controller input structure through a process superstructure formulation that enables the adaptive utilisation of the most suitable set of manipulated variables based on the prevailing operating conditions. A generalised framework of this flexible controller type along with a nonlinear dynamic model for the plant accounting for the simultaneous satisfaction of stringent control objectives on the effluent quality and the GHG minimisation is developed. The proposed controller incorporates manipulated variables for all admissible aeration intensities, internal flow recirculation streams, external carbon sources, influent flow distribution in each bioprocessing unit, unit volume variations and recirculation flow percentage. Accurate simulations indicate the achievement of a superior emission reduction performance compared to state-of-the-art MPC implementations in WWTP. Every consideration of a manipulated variable set is associated with respect to its contribution to the total GHG reduction for each mode of operation.

1. Introduction

Due to the constantly increasing demand in water usage for industrial and urban operations, WWTP are targeted to operate under more stringent operating specifications. To successfully biometabolise the wastewater and achieve acceptable effluent water quality, the WWTP system needs to be constantly monitored and efficiently controlled. The biochemical reactions as contributors of GHG emissions have been properly named as "On-Site" Emissions. Additionally, process equipment that are being deployed to control the plant also contribute to a significant degree to the overall GHG emissions. Those are called the "Off-Site" emissions, which result mainly from the aerator and pump operations.

The main challenges associated with the efficient control of WWTPs are:

- High variability of the operating conditions and the external inputs in the system (e.g., influent load variation due to abrupt weather changes).
- Nonlinearity of the process system dynamics.

- An abundance of unmeasured state variables that are important to describe the system behaviour (1).
- Uncertainty of model parameters, especially those related to the growth rate of microorganisms and indicated in the work of Henze et al. (1987) and later enhanced by Alex et al. (2008).

Current state-of-the-art literature is limited to control approaches that use specific manipulated variables. A common choice is the manipulation of the aeration intensity and recirculation flow in the aerator. Vega et al. (2014) considered such a choice for the manipulated variables and employed a simplified plant configuration consisted of two-units chamber. Zeng and Liu (2015) used a similar approach with the Benchmark Simulation Model 1 (BSM1) plant configuration suggested by Alex et al. (2008). In Han and Qiao (2014) a similar input controller structure is utilised in a MPC, which is complemented by a neural network structure that performs online approximation of the system's states. In Stentoft et al. (2021), the on-off durations of aerator operation are controlled. In Huang et al. (2020), the manipulated variables are the aeration intensities of chambers 3, 4 and 5 (Figure 1). In Sweetapple et al. (2014a), the input variables involved the internal recirculation flow, wastage flow, aeration intensities of chambers 1 and 2, and the external carbon sources of chambers 1, 2 and 5. To the best of the authors' knowledge, there is no published work that addresses WWTP control through a flexible approach that allows the potential use of all available degrees of freedom in the process system. There is, however, a study wherein the sensitivity of the available manipulated variables is investigated (Sweetapple et al., 2014b), that identified the aeration intensities as the most influential factors with regards to GHG emissions, a conclusion that agrees with observations made in the scope of this work. In the current study, the deployment of all feasible manipulated variables is considered to enable the greatest possible flexibility in the control scheme at every time instance. The main control objective is the minimisation of the GHG emissions and operating costs, while maintaining the effluent quality within allowable limits.

Due to the constant increase in computing power, it is now possible to use complex optimisation algorithms in industrial settings. Especially in the case of WWTPs, where time constants are in the order of magnitude of approximately 15 min, it is realistic to efficiently use conventional non-linear optimisation algorithms in real-time. In addition, high stiffness of the model differential equations, as WWTP systems encompass process dynamics that are characterised by a large range of temporal scales, result in the need of efficient temporal decomposition techniques. For instance, the control of Dissolved Oxygen (DO) requires a different time scale than the control of ammonia and nitrate in the sludge (Weijers, 2000). There have been significant efforts towards temporal decomposition of the WWTP dynamics over the past two decades. The proposed approach aims also to provide a highly performing NMPC (Nonlinear MPC) leveraging the multiple control objectives.

2. Process system and manipulated variables' configuration description

In this work, the objective function is consisted of a term for the generated GHG emissions, terms for the manipulated variable variations, terms for state tracking errors between different levels of controller operation, and a term for the Effluent Quality Index (EQI), which is a weighted average of effluent component loads that have significant influence on the quality of effluent flow water and are usually considered to satisfy regional regulations (Alex et al., 2008). As far as the relative importance between each optimisation term is concerned, an extensive analysis in multi-objective optimal control is provided in Stentoft et al. (2021).

As an accelerator of nature's processes, WWTP goal of operation is to achieve fast and effective elimination of toxic nutrients in wastewater. Among the different biological treatment methods, Activated Sludge Process (ASP) is usually selected. Inside the unit chambers of the WWTP (Figure 1), oxidation of the inserted biomass and denitrification occur in aerated and anoxic conditions.

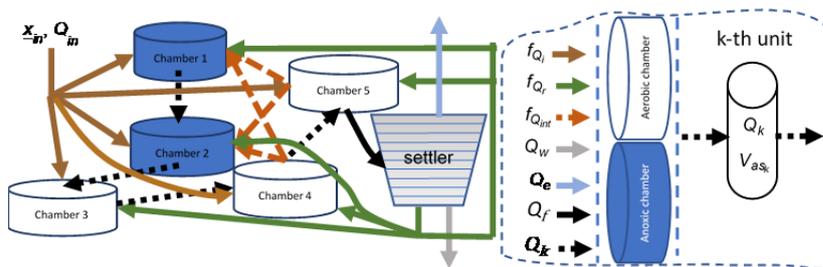


Figure 1: Network diagram depicting the flow inputs, outputs and recirculations (arrows). Right-most shape of Figure: notation for unit chamber k . Q_k and V_{as_k} refer to the flow rate and volume of the k -th chamber. Q_{in} is the influent flow rate, which can split to the f_{Q_i} fractions

The plant configuration is described by two anoxic and three aerobic chambers, followed by a 10-layer non-reactive secondary clarifier as shown in Figure 1. A generally preferred model that provides a good compromise between dynamics accuracy and computational effort is the BSM1 model (Alex et al., 2008) and

is used in this work. The manipulated variables shown in Eq(1) involve the flow rates, aeration intensities and unit chamber volumes.

$$\underline{u}^T = \left[\underline{u}_{KLa}^T, \underline{u}_{f_{Q_i}}^T, \underline{u}_{f_{Q_{int}}}^T, \underline{u}_{Q_{EC}}^T, \underline{u}_{V_{as}}^T, \underline{u}_{f_{Q_r}}^T, Q_w \right] \quad (1)$$

$$\text{where: } \underline{u}_{var_i}^T = \left[var_{i_1}, \dots, var_{i_{n_u}} \right], \text{ } var = \{KLa, f_{Q_i}, Q_{EC}, V_{as}, f_{Q_r}\}, \underline{u}_{f_{Q_{int}}}^T = \left[f_{Q_{int_1,1}}, \dots, f_{Q_{int_1,n_{anox}}}, \dots, f_{Q_{int_{naer,n_{anox}}} \right]$$

KLa denotes the aerator-actuated aeration intensities or oxygen transfer (i.e., the oxygen flow rate that is transferred to the microbial cultures to be biometabolised) applied to each unit chamber. Variables f_{Q_i} , f_{Q_r} , $f_{Q_{int}}$ and Q_w represent the influent flow rate, external recycle rate, internal recycle rates and wastage flow, respectively (Figure 1). $Q_{EC,k}$ represents the pump actuated supplementary biodegradable external carbon source flow for the k-th unit chamber which facilitates denitrification. The time-dependent state vector ($\underline{x}(t) \equiv \underline{x}_t$) is defined as:

$$\underline{x}^T = \left[\underline{x}_1^T, \dots, \underline{x}_{n_u}^T, \underline{x}_{still}^T \right] \text{ (Time index is omitted for simplicity)}$$

The state vector (\underline{x}_k) that describes the k-th unit chamber is given below.

$$\underline{x}_k^T = \left[S_{I_k}, S_{S_k}, X_{I_k}, X_{S_k}, X_{BH_k}, X_{BA_k}, X_{P_k}, S_{O_k}, S_{NO_k}, S_{NH_k}, S_{ND_k}, X_{ND_k}, S_{ALK_k} \right], 1 \leq k \leq n_u \quad (2)$$

In the above-given vector, the elements that start with "S" represent the soluble components, whereas those with "X" represent the insoluble components. For example, S_O represents the soluble oxygen concentration in the flow of the k-th chamber. A similar structure is used for the influent flow \underline{x}_{in} (Figure 1). The state vector (\underline{x}_{still}) that describes the settler is given below.

$$\underline{x}_{still}^T = \left[\underline{x}_{XTSS}^T, \underline{x}_{S_i}^T, \underline{x}_{S_s}^T, \underline{x}_{S_o}^T, \underline{x}_{S_{NO}}^T, \underline{x}_{S_{NH}}^T, \underline{x}_{S_{ND}}^T, \underline{x}_{S_{ALK}}^T, \underline{x}_{solids_u}^T \right]$$

$$\text{where: } \underline{x}_{var}^T = [var_1, \dots, var_{n_L}], \text{ } var = \{ "XTSS", "S_I", "S_S", "S_O", "S_{NO}", "S_{NH}", "S_{ND}", "S_{ALK}" \}$$

and $\underline{x}_{solids_u}^T = [X_{I_u}, X_{S_u}, X_{BH_u}, X_{BA_u}, X_{P_u}, X_{ND_u}]$, u: refers to underflow: $Q_u = Q_f - Q_e$ (Figure 1). X_{XTSS} is the total solid concentration in the i-th settler layer which is equal to $0.75 \cdot (X_I + X_S + X_{BH} + X_{BA} + X_P)$.

BSM1 (Alex et al., 2008) is the basis for the formulations of the nonlinear differential state equations, derived from mass flow balance equations for the five unit chambers, i.e. 13 equations for each chamber, and the 10-layered non-reactive settler (the number of settler equations is equal to three related to the first three elements of \underline{x}_{still}^T of Eq(2)). The mass balance equations also include terms that represent the growth and decay of biochemical components that take place inside the unit chamber due to reaction kinetics, as per Activated Sludge Model 1 (ASM1) (Henze et al., 1987). Certain additions to the state equations of the BSM1 model are considered, to account for the added flexibility of the controller, which include extra flow inputs and outputs to unit chambers that arise from the potential flow recirculations (Figure 1). Each arrow in Figure 1 that points to and from a chamber essentially represents a mass flow that has to be added in the state equations. No modification is required for the settler equations that can be found in Alex et al. (2008). All the biochemical components in the state vectors will be considered as known (i.e., perfectly estimated).

Table 1: Relationship between measurable variables and state variables in a unit chamber (table obtained from Yin and Liu, 2018). $T_1 = X_S + X_I + X_{BA} + X_{BH}$, conc.: concentration

Measurement	State expression	Measurement	States' expression
Oxygen Conc.	S_O	Alkalinity Conc.	S_{ALK}
Conc. of NH_4^+ & NH_3	S_{NH}	COD	$BOD + T_1$
Conc. of nitrate & nitrite oxygen	S_{NO}	BOD	$S_S + S_I$
Conc. of suspended solids	$T_1 + X_P + X_{ND}$		

3. Methods

The nonlinear features of the BSM1 are fully included in the MPC, since linearisation of the model equations results in significant performance deterioration (Vega et al., 2014). To calculate the GHG emissions a combination of the BSM1, ASM1 and Bridle's model is implemented, a choice that is also considered in Huang et al. (2020). An analytic representation of the calculations can be found in Snip (2010).

The employed optimisation package is the open-source symbolic-numerical solver CasADi (Andersson et al., 2019). The discretisation method used is the direct collocation method. The MPC related parameters are given in Figure 2. The external disturbance is the influent flow load (i.e., flow rates) and component concentrations of the components that correspond the chamber's state vector \underline{x}_k in Eq(2). A premeasured influent dataset in Alex et al. (2008) was utilised that corresponds to stormy weather conditions ("STORMINFLUENT" dataset of Alex et al. (2008)). For this work, it is assumed that the influent flow signals are correctly identified and forecasted. Similarly, to Huang et al. (2020), this work considers the following sources of GHG emissions: endogenous decay, BOD removal, nitrification, denitrification, sludge disposal, aeration, pumping and chemical usage. Other researchers such as Stentoft et al. (2021) consider as GHG sources those attributed to nitrous oxide emissions and electricity consumption.

3.1 Temporal Decomposition

The temporal decomposition problem is not yet solved by any closed-loop method and has been tackled by several authors in a heuristic manner. The timescale properties of the reaction kinetics model (ASM1) are not very well understood (Weijers, 2000). A representation of the dynamics in different time scales is presented in Weijers (2000). The proposed controller structure is a two-staged NMPC, as depicted in Figure 2.

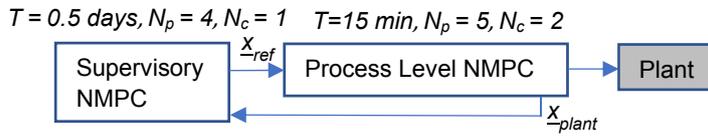


Figure 2: Simplified outline of the controller - System architecture. The sampling time of each NMPC controller is denoted as T and the prediction and control horizons as N_p and N_c

The supervisory NMPC solves the state equations in steady state and minimises the GHG emissions. The reactions can be assumed as static for large time scales and this module further utilises weather data forecasts that are in essence generated by a sliding window of the initial premeasured raw weather data for a time window of 0.5 d. For the scope of this work, it will be assumed that the influent signal is correctly predicted, by applying the aforementioned smooth signal and incorporating measurement disturbances in the future. The process level NMPC aims to implement the outcome of the supervisory level controller and further satisfy the quality specification of the effluent stream.

3.2 Objective Functions

The generic form of the MPC objective function is given below.

$$J_t = \sum_{j=0}^{H-1} \left(\left(\underline{x}_{t+j,t} - \underline{x}_{ref,t+j,t} \right)^T M \left(\underline{x}_{t+j,t} - \underline{x}_{ref,t+j,t} \right) + \underline{u}_{t+j,t}^T Q \underline{u}_{t+j,t} + f_{GHG} \left(\underline{x}_{t+j,t}, \underline{u}_{t+j,t} \right) + f_{EQI} \left(\underline{x}_{t+j,t}, \underline{u}_{t+j,t} \right) + f_{eff_Qual_viol} \left(\underline{x}_{t+j,t}, \underline{u}_{t+j,t} \right) \right) \quad (3)$$

The supervisory NMPC does not contain a state-tracking error penalty, first term of Eq (3), whereas the process level NMPC considers it, because it is dictated by the supervisory controller. Eq(4) represents the penalty of exceeding the legislation-mandated effluent index (or discharge) limits, see Eq(5).

$$f_{eff_Qual_viol}(\underline{x}, \underline{u}) = \sum_{i=1}^5 \begin{cases} 0, & (x_{eff})_i \leq (x_{eff,lim})_i \\ w_{eff_i}, & (x_{eff})_i > (x_{eff,lim})_i \end{cases} \quad (4)$$

$$\underline{x}_{eff}^T = [N_{tot,eff}, COD_{eff}, S_{NH,eff}, X_{TSS,eff}, BOD5_{eff}] < \underline{x}_{eff,lim}^T = [18, 120, 4, 30, 10] \text{ g/m}^3 \quad (5)$$

4. Results and discussion

The simulations yielded GHG emissions (Figure 3b, wherein kg CO₂ eq. represents the equivalent CO₂ yield from the various generated greenhouse gases) that are low for WWTP standards, given the specific discharge limits in Eq(5)(4). The only manipulated variables that the supervisory MPC optimises are the unit chamber volumes, since it is not realistic to variate them with the rate dictated by the process level MPC's sampling rate (Figure 2). By observing Figure 4 it becomes apparent that the controller indeed chooses to variate the available manipulated variables at different time instances. For presentation simplicity, only the aeration intensities for the chambers 4 and 5 are shown. The variables that experience the largest levels of utilisation by the controller are the aeration intensities and the external carbon sources (Figure 4). For the influent flow

split it was assumed that $f_{Q_{r1}}=1$ and $f_{Q_{rk}}=0$ for $k>1$, since toxic influent compound concentrations such as S_{NH} need to be biodegraded so that the respective concentrations in the effluent flow remain below discharge limits. By observing Figure 5d, it becomes apparent that the consideration of all aeration intensities as manipulated variables leads to an increase in the aeration energy. This is expected since additional aeration energy is required to variate the aeration intensities. The effluent quality related components are depicted in Figure 5. Effluent indexes are mostly kept below limits and $BOD_{5_{eff}}$ exceeds the limit at time periods that correspond to the most severe influent load peaks. Compared to Huang et al. (2020), all values of effluent quality indexes computed in the present work are lower, except for $BOD_{5_{eff}}$. The GHG emissions are reduced to a factor of 2.6 in the present work compared to the ones in Huang et al. (2020) and to a factor of 5 compared to the ones in Kim et al. (2015). However, the effluent indexes in Kim et al. (2015) are maintained at lower levels (specifically $S_{NH_{eff}}$, which is kept around 2 g/m^3). This observation indicates that minimisation of GHG emissions can compromise the minimisation of the values in x_{eff} (Eq.(5)). In Stentoft et al. (2021), the lowest GHG emissions were around 65 kg/day , which are generated from N_2O production and electricity consumption and are approximately 15 times smaller than the corresponding ones computed in the present work. However, direct comparison of GHG emissions in this case is difficult, since the plant configuration in Stentoft et al. (2021) is very different in terms of number of unit chambers and corresponding volumes. As stated in Fighir et al. (2019) expert user knowledge is required when comparing output data between different WWTPs.

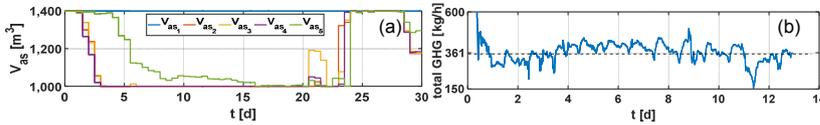


Figure 3: Optimal unit chamber volumes (a) and total GHG concentrations (in $\text{kg CO}_2\text{-eq./h}$) (b)

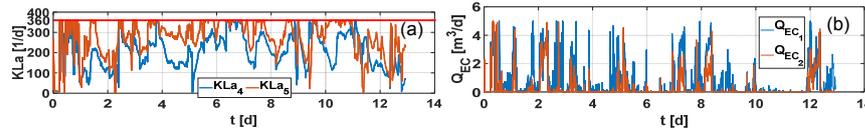


Figure 4: (a) Optimal aeration intensities (units 4 and 5), (b) Optimal external carbon source flows (units 1 and 2)

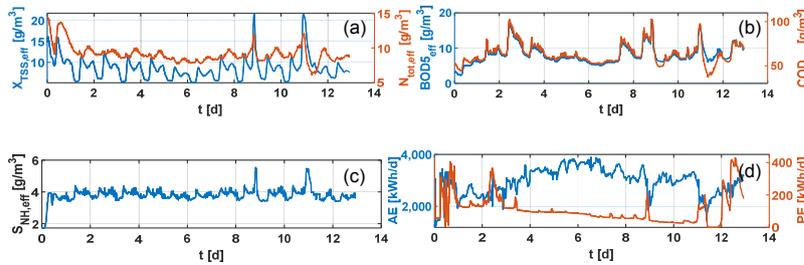


Figure 5: Effluent Quality signals (a-c) and Aeration and Pumping Energies (d)

5. Conclusions

The consideration of a flexible WWTP model with regards to the manipulated variables provides superior results compared to schemes that employ a limited number of manipulated variables and similar plant configurations found in recent literature. The proposed approach is computationally efficient and allows for the implementation of the control system under real-time conditions, through the utilisation of conventional non-linear optimisation packages.

Nomenclature

$BOD_{5_{eff}}$ – Effluent biochemical oxygen demand, g/m^3

COD_{eff} – Effluent chemical oxygen demand, g/m^3

$f_{Q_{int}}$ – Internal recirculation fraction, m^3/d

f_{Q_r} – External recirculation fraction

KLa – Aeration intensity, $1/\text{d}$

n_{aer} – Number of aerated chambers

n_{anox} – Number of anoxic chambers

NH_3 – Ammonia

NH_4^+ – Ammonium	V_{as} – Activated sludge unit chamber volume, m^3
N_{tot} – Total nitrogen concentration, g/m^3	X_{BA} – Active autotrophic biomass concentration, g/m^3
n_u – Number of unit chambers	X_{BH} – Active heterotrophic biomass concentration, g/m^3
Q_{EC} – External carbon source flow rate, m^3/d	X_I – Particulate inert solid matter concentration, g/m^3
Q_w – Wastage flow rate, m^3/d	X_{ND} – Particulate biodegradable organic nitrogen concentration, g/m^3
S_{ALK} – Alkalinity concentration, g/m^3	X_P – Particulate products arising from biomass decay concentration, g/m^3
S_I – Soluble inert organic matter, g/m^3	X_S – Slowly biodegradable substrate concentration, g/m^3
S_{ND} – Soluble biodegradable organic nitrogen concentration, g/m^3	$X_{TSS_{eff}}$ – Total effluent solid concentration, g/m^3
S_{NH} – NH_4^+ & NH_3 nitrogen concentration, g/m^3	$(\blacksquare)_{eff}$ – Variable that refers to the effluent flow
$S_{NH,eff}$ – Effluent S_{NH} , g/m^3	(\blacksquare) – Vector variable
S_{ON} – Nitrate and nitrite nitrogen concentration, g/m^3	$(\blacksquare)_i$ – i-th element of vector
S_O – Soluble oxygen concentration, g/m^3	
$S_{O,sat}$ – Saturation S_O	
S_S – Readily biodegradable substrate concentration, g/m^3	
\underline{u} – Vector of manipulated variables	

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References

- Alex J., Benedetti L., Copp J., Gernaey K.V., Jeppsson U., Nopens I., Pons M.N., Rieger L., Rosen C., Steyer J.P., Vanrolleghem P., Winkler S., 2008. Benchmark Simulation Model no. 1 (BSM1), <<https://www.iea.lth.se/publications/Reports/LTH-IEA-7229.pdf>>, accessed 16/09/2021.
- Andersson A.E.J., Gillis J., Horn G., Rawlings B.J., Diehl M., 2019, CasADi: a software framework for nonlinear optimization and optimal control. *Math. Prog. Comp.*, 11, 1–36.
- Figdor D., Teodosiu C., Fiore S., 2019, Environmental and Energy Assessment of Municipal Wastewater Treatment Plants in Italy and Romania: A Comparative Study, *Water*, 11(8), 1611.
- Han H.G., Qiao J.F., 2014, Nonlinear Model-Predictive Control for Industrial Processes: An Application to Wastewater Treatment Process, *IEEE Transactions on Industrial Electronics*, 61(4):1970-1982.
- Henze M., Grady C.P.L. Jr., Gujer W., Marais G.v.R., Matsuo T., 1987, Activated Sludge Model No.1. International Association on Water Pollution Research and Control - Scientific Technical Reports No.1.
- Huang F.N., Shen W.H., Zhang X.W., Seferlis P., 2020, Impacts of dissolved oxygen control on different greenhouse gas emission sources in wastewater treatment process, *Journal of Cleaner Production*, 274, 123233.
- Kim D., Bowen J.D., Ozelkan E.C., 2015, Optimization of wastewater treatment plant operation for greenhouse gas mitigation, *Journal of Environmental Management*, 163, 39-48.
- Snip L., 2010, Quantifying the greenhouse gas emissions of wastewater treatment plants. PhD Thesis Systems and Control, University of Wageningen, The Netherlands.
- Stentoft P.A., Munk-Nielsen T., Møller J.K., Madsen H., Valverde-Pérez B., Mikkelsen P.S., Vezzaro L., 2021, Prioritize effluent quality, operational costs or global warming? –Using predictive control of wastewater aeration for flexible management of objectives in WRRFs. *Water Research*, 196, 116960.
- Sweetapple C., Fu G.T., Butler D., 2014a, Identifying sensitive sources and key control handles for the reduction of greenhouse gas emissions from wastewater treatment, *Water Research*, 62, 249-259.
- Sweetapple C., Fu G.T., Butler D., 2014b, Multi-objective optimisation of wastewater treatment plant control to reduce greenhouse gas emissions, *Water Research*, 55, 52-62.
- Vega P., Revollar S., Francisco M., Martina J.M., 2014, Integration of set point optimization techniques into nonlinear MPC for improving the operation of WWTPs, *Computers & Chemical Eng.*, 68, 78-95.
- Weijers, S., 2000, Modelling, Identification and Control of Activated Sludge Plants for Nitrogen Removal. PhD Thesis, TU Eindhoven, The Netherlands.
- Yin X.Y., Liu J.F., 2018, State estimation of wastewater treatment plants based on model approximation, *Computers and Chemical Engineering*, 111, 79–91.
- Zeng J., Liu J.F., 2015, Economic Model Predictive Control of Wastewater Treatment Processes, *Industrial & Engineering Chemistry Research*, 54 (21), 5710–5721.