Plant-wide modelling and simulation using steady-state data: a case study of the Gliwice WWTP, Poland

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Abstract

In last decade the focal point of the activated sludge (AS) modelling shifted from a secondary-treatment to a plant-wide level. This new approach offers more possibilities, therefore demands more effort and expertise from a modeller.

This paper presents a plant-wide approach to modelling and simulation of a full-scale AS wastewater treatment plant (WWTP). The construction and routine operational data of the full-scale Central WWTP in Gliwice (Poland) were used in this study to develop an integrated model of the water and sludge lines of the plant. The core of the plant model was the Activated Sludge Model No.1 (ASM1), which combined with sub-models of the other processes, was implemented in the WEST® Software version 3.7.6. The calibration strategy, verification and predictive capacity of the model are discussed. The calibrated model permitted acceptable accuracy of the simulation, yet limited data restrained its scope. Thus, the obtained mathematical description of the plant is a preliminary yet sound basis for a more versatile model. The model limitations and opportunities for its further applications and development are discussed.

Key words: computer simulation, mathematical modelling, plant-wide model, sludge treatment, wastewater treatment

INTRODUCTION

One of the newest trends in modelling wastewater treatment processes is to develop models describing the behaviour of water and sludge lines in wastewater treatment plants (WWTPs), not merely the secondary treatment processes (Grau et al. 2007). Simulation performed using an integrated model of the entire plant (a plant-wide model) permits to develop an optimal control strategy and control of activated sludge (AS) process and increase the efficiency of wastewater treatment while reducing operating costs. It should be noted that the optimal strategy for the operation of the WWTP, taking into account the interaction between the various processes in the wastewater and sludge, is not always the optimal strategy for unit processes. For this reason, a comprehensive optimization of AS system requires development of a model that links the processes of mechanical and biological wastewater treatment and sludge processing (Grau et al. 2007). The main challenges of plant-wide modelling stem from the fact that models of individual unit processes have different sets of state variables and often cannot be directly coupled. There are certain solutions to this problem: to create a
‘supermodel’ containing variables of all models, to develop interfaces linking variables of models, or to use simplistic models, which could be easily coupled with models of focal processes (Volcke et al. 2006). Similarly to modelling less complex systems, a dynamic simulation may be preceded by a steady-state simulation. To this end, monthly averaged typically available construction and operational data can be used. A static calibration is very useful procedure, prior to a dynamic calibration, however model calibrated via steady state calibration applied to model dynamic process scenarios may perform inaccurately. This may the case when real input variations are faster than the slow process dynamics resulting from the steady state calibration. Generally in a steady-state calibration only parameters responsible for a long-term performance can be determined (Volcke et al. 2006).

The general objective of this study was to investigate the possibility of using mathematical models of various wastewater and sludge treatment processes to mimic the behaviour of the Central Wastewater Treatment Plant in Gliwice, Poland, including its wastewater and sludge trains, based on steady-state data. More specifically, the goals of this modelling study were prediction of volatile suspended solids (VSS) concentration in the aerobic digester and daily biogas production.

**METHODS**

**Description of the Gliwice WWTP**

The WWTP investigated in this study is located in the city of Gliwice (Poland) and it is the central WWTP of the city. This WWTP receives wastewater from the city area, which is populated by 200,000 people. The wastewater is collected and conveyed to the WWTP by the sewer system, which is largely a separate sewer with a total length of about 400 km. It was estimated that up to 10% of the influent flow is of industrial origin: chemical, mining and plastics manufacturing industries. The treated effluent is discharged into the Kłodnica River (Przedsiębiorstwo Projektowo-Inżynieryjne EKOLOG 2000; Sikora 2003).

The preliminary and primary treatment units include: screening, two aerated vertical grit chambers and three circular primary settlers (volume \( V_{PC} = 763 \text{ m}^3 \), water head \( H_{PC} = 3 \text{ m} \), diameter \( D_{PC} = 18 \text{ m} \)). The secondary treatment takes place in three parallel trains, to which wastewater is evenly distributed. A single train of secondary treatment contains a series of AS tanks (in downstream order): pre-denitrification tank (PD, volume \( V_{PD} = 700 \text{ m}^3 \)), anaerobic tank (AN, volume \( V_{AN} = 700 \text{ m}^3 \)) and aerobic-anoxic tank (N-DN, anoxic volume \( V_{DN} = 4,260 \text{ m}^3 \), oxic volume \( V_{N} = 4,615 \text{ m}^3 \)). The AN tank and PD tank are identical in terms of their construction, which are rectangular tanks adjacent to their long sides and interconnected by a demersal conduit. The content of each tank is mixed and kept in suspension by low-speed agitators. The N-DN tank is a rectangular basin with short sides rounded permitting circular flow of wastewater in a carousel-like fashion. Inside the tank there is a longitudinal partition wall with semicircular baffles at each end. Such configuration, resembling a race track, facilitates optimal conditions for circular flow. The mixed liquor of N-DN tank is aerated by six draft tubes. Due to significant working depth of the reactor the aeration and circulation is enhanced by two low-speed propellers. The conditions occurring within the confines of the N-DN tank are simultaneously aerobic and anoxic contingent on the zone of the reactor, aeration intensity and wastewater quality and quantity. The varying interplay of these conditions affects nitrification and denitrification efficiency in the reactor. Mixed liquor suspended solids (MLSS) are separated from the treated effluent in three secondary settlers (volume \( V_{SC} = 5,724 \text{ m}^3 \), water head \( H_{SC} = 5.05 \text{ m} \), diameter \( D_{SC} = 38 \text{ m} \)).

Sludge handling units of the investigated WWTP are used for processing of primary and secondary sludge. Sludge thickening is performed in gravity thickeners for primary sludge (hydrolysis and release...
of volatile fatty acids) and mechanical thickeners for secondary sludge. After thickening, sludge undergoes mesophilic anaerobic digestion in two digesters (volume $V_D = 2,851 \text{ m}^3$, active height $H_{SC} = 17.2 \text{ m}$, diameter $D_D = 14.6 \text{ m}$). Digested sludge is dewatered with filter presses and then disposed of at approved locations.

The plant was designed for the removal of organic matter, nitrogen by simultaneous denitrification nitrification and phosphorus by biological dephosphatation and chemical precipitation with iron salts.

For the simulation study only routine operational data from the Gliwice plant were used; no additional measurements were performed. The raw data collected from the plant were examined to extract several sets of data representing approximately 30-d periods of steady state operation. These data were elaborated and averaged, assuming that this average represents steady state. The average data from two different periods were used in this simulation study for model calibration (Table 1) and for verification of the calibrated model.

### Table 1 | Operational and performance characteristics of the Central Gliwice WWTP in the calibration period

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Influent flow rate</td>
<td>m$^3 \text{ d}^{-1}$</td>
<td>32,995</td>
</tr>
<tr>
<td>MLSS$^a$</td>
<td>g L$^{-1}$</td>
<td>4.9</td>
</tr>
<tr>
<td>Return sludge ratio</td>
<td>% of Q</td>
<td>1.65</td>
</tr>
<tr>
<td>Temperature</td>
<td>°C</td>
<td>10.5</td>
</tr>
<tr>
<td>Waste sludge flow rate</td>
<td>m$^3 \text{ d}^{-1}$</td>
<td>808</td>
</tr>
<tr>
<td>RAS$^b$</td>
<td>g L$^{-1}$</td>
<td>5.9</td>
</tr>
<tr>
<td>DO$^c$ in the aerobic zone</td>
<td>mg L$^{-1}$</td>
<td>0.5</td>
</tr>
<tr>
<td>Concentration of:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>COD$_{tot}^d$</td>
<td>mg L$^{-1}$</td>
<td>469.6</td>
</tr>
<tr>
<td>Total Kjeldahl Nitrogen (TKN)</td>
<td>mg L$^{-1}$</td>
<td>70.6</td>
</tr>
<tr>
<td>Ammonia nitrogen (N-$\text{NH}_4$)</td>
<td>mg L$^{-1}$</td>
<td>44.7</td>
</tr>
<tr>
<td>Nitrate nitrogen (N-$\text{NO}_3$)</td>
<td>mg L$^{-1}$</td>
<td>2.1</td>
</tr>
<tr>
<td>Total Suspended Solids (TSS)</td>
<td>mg L$^{-1}$</td>
<td>213.3</td>
</tr>
</tbody>
</table>

$^a$Mixed liquor suspended solids.
$^b$Return activated sludge.
$^c$Dissolved oxygen.
$^d$Total chemical oxygen demand.

### Simulation environment

In this work simulations were carried out in the WEST® (World Wide Engine for Simulation, Training and Automation) Software Package version 3.7.6 (Vanhooren et al. 2003). The WEST® simulator was chosen as a modelling and simulation environment because of the in-house experience, direct application to WWTP and possibility to reuse previously developed models.

### Model configuration

The integrated model of the WTTP under study was based on a model of secondary treatment processes occurring in the real-world system. Models of primary treatment and sludge line processes were added to the model of a biological treatment in water line, which was previously modelled and calibrated. Input variables are qualitative and quantitative characteristics of raw wastewater of the WWTP in Gliwice. Contaminants load following from recycling of reject water from sludge processing into water line is included in raw wastewater properties. Thus, modelling of reject waters
impact on wastewater treatment was omitted in this study. The main components of the proposed model are (Figure 1):

- Primary settling: primary point settler (Most for Water 2007); non-reactive settler;
- Four-reactor AS process based on Activated Sludge Model No.1 (ASM1) (Henze et al. 1987) in CSTR reactors; Arrhenius equation was used to account for temperature variations;
- Secondary settler based on Takacs model (Takács et al. 1991), non-reactive settler;
- Sludge thickening based on Efficiency Thickener model (Most for Water 2009); ideal and continuous process; non-reactive; the same model was used both for gravity and mechanical thickening;
- Anaerobic digestion based on the Desjardins and Lessard model (Desjardins & Lessard 1992).

In terms of hydrodynamics, the PD and AN tanks were represented by a single CSTR tank reactor, each, and the circular N-DN tank was represented by a tank-in-series model comprising two CSTRs. The number of tanks in series was estimated based on the results of simulation with various numbers of tanks.

AS process was modelled using ASM1 as it may be easily interfaced with the other submodels, in particular, the anaerobic digestion model. The ASM1 permits to simulate organic matter and nitrogen removal in the AS process. F-C (flux-concentration) and C-F (concentration-flux) converters were used during computer simulation because all the models in WEST are expressed in terms of fluxes and model input and output are expressed in terms of concentrations (Most for Water 2007). A model
of proportional-integral (PI) controller was used for the DO control in the N Tank by manipulation of the oxygen transfer coefficient, \(K_{La}\). In the PI model, the value of the manipulated variable changes proportional to the value of the error signal and to the value of the integral of the error function in time (Most for Water 2007). The Loop breaker model was used to accelerate the simulation performance.

**Influent fractionation**

An application of the ASM1 requires the influent characterization on a COD\(_{tot}\) basis, which is then split into a variety of fractions according to the model variables (see Henze et al. 1987). For the modelling purposes, the operational routine data of the Gliwice plant were used. In order to generate the model influent, a conversion of the conventional plant parameters described by raw wastewater concentrations was performed for the ASM1 model components. Influent wastewater fractionation procedure proposed in Mąkinia et al. (2002) was employed in this study. The concentrations of nitrogenous components of ASM1 were calculated using the formulae proposed in Vanhooren and Khanh (1996).

**Sensitivity analysis**

Sensitivity analysis was performed based on steady-state simulations, in accordance with the one-variable-at-a-time approach (Melcer et al. 2003; Mikosz 2009; Mąkinia 2010). In the first step of the algorithm a simulation was performed with default values of the model. Then the value of each parameter was individually increased by 10% of the default value and then after another simulation new values of state variables were obtained. The results of sensitivity analysis allowed discrimination between relatively less sensitive and the most sensitive variables, which consequently were adjusted to calibrate the model (Vanrolleghem et al. 2003). Sensitivity analysis was carried out only for the biokinetic model.

**Calibration and verification of the model**

The predictions of the model for effluent quality, biogas production, as well as input sludge concentration in the digester were used as a measure for the model accuracy of representing the plant performance. The initial parameters of the model were based on the default values suggested in Henze et al. (1987) for the ASM1 submodel or the values default in the WEST Software for the other submodels. Calibration strategy involved the adjustment of the model parameters in order to minimize the discrepancies between the model output and the observed data. The results of the simulation with the default model values did not fit the real data with an acceptable accuracy. To increase the predictive power of the simulations the model calibration was carried out.

Sedimentation model of the secondary settling tank is an integral part of the secondary treatment model and may be subjected to calibration if needed. In the case of the secondary clarifier model one of the most important output variables is TSS concentration in its effluent. The proper operation of the secondary clarifier model not only determines the correct TSS concentration predictions, but also affects the values of other model variables that describe the composition of the wastewater discharged to the receiver. During the calibration of sedimentation model the values of two parameters were adjusted. The non-settleable fraction \(f_{ns}\) coefficient was decreased compared to the default value, this is, from 0.00228 to 0.00100, respectively. This allowed reduction of the content of non-settleable organic fraction of TSS in the excess sludge. The value of the settling parameter for the low concentrations \(r_P\) was from 0.00286 to 0.00700 m\(^{-3}\) g\(^{-1}\), thus improving the conditions of sedimentation in the zone of clarification in the secondary settler. The adjusted values are comparable with the
literature data (Takács et al. 1991). The calibration improved the settling properties of the sludge and increased predicting power of the model in terms of TSS concentration in the outflow. The necessity to modify the default parameter values may result from the effect of partial flocculation of the sludge by polyelectrolytes, which together with the reject waters are recycled into the wastewater line. In order to increase the predictive power of the biokinetic model and the overall plant model the following ASM1 stoichiometric and kinetic parameters were adjusted: $Y_{1H}$, $\mu_{A}$, $b_{A}$, $K_{O,H}$, $K_{NH}$, $k_{A}$, $k_{H}$. The parameters values adopted during the calibration phase are within the range reported in the literature (Henze et al. 2000; Melcer et al. 2003; Makinia 2010). The heterotrophic yield coefficient ($Y_{1H}$) adjusted from 0.67 to 0.75 gCOD·(gCOD)\(^{-1}\) allowed increasing the concentration of MLSS and RAS. The ASM1 model does not allow storage of endogenous organic matter, so the need to increase the default value of the coefficient of $Y_{1H}$ can indicate the use of endogenous substances for the growth of heterotrophs (Makinia 2010). The autotrophic maximum specific growth rate ($\mu_{A}$) coefficient was increased from 0.8 to 1.2 d\(^{-1}\), which enhanced the nitrification rate and thus lowering the concentration of N-NH\(_4\) in the effluent. The elevated value of $\mu_{A}$ may stem from the presence of nitrifiers with higher affinity to the substrate and thus increased growth rate compared to the default model values. The autotrophic decay rate coefficient ($b_{A}$) was reduced from 0.2 to 0.1 d\(^{-1}\), which resulted in increased concentrations of active biomass of nitrifying bacteria and eventually led to a lower concentration of N-NH\(_4\) in the effluent. The adjustment of $b_{A}$, as in the case of $\mu_{A}$, may be due to particularities of the nitrifiers. The oxygen half-saturation coefficient for heterotrophs ($K_{O,H}$) was increased from 0.2 to 0.4 gO\(_2\) m\(^{-3}\), thereby decreasing N-NO\(_3\) in the effluent, mainly due to increased threshold oxygen concentration at which switching between anoxic and oxic metabolism occurs. The adjusted value of $K_{O,H}$ is relatively high, compared to the values presented in the literature (Henze et al. 2000), which indicates the existence of oxygen transfer limitations within the flocs (e.g. caused by filamentous bacteria or polyelectrolytes). As in the case of $K_{O,H}$ also the ammonia half-saturation coefficient for autotrophs ($K_{NH}$) is contingent on the efficiency of N-NH\(_4\) diffusion into the AS flocs. Its value, however, was decreased markedly from 1.00 to 0.06 gN-NH\(_4\) m\(^{-3}\), which allowed reducing the concentration of N-NH\(_4\) in the effluent. The relatively small value of $K_{NH}$ can be explained by hydrodynamic conditions in the reactor or increased affinity of the nitrifiers to the substrate, or both. It is noteworthy that the value of $K_{NH}$ increases with a decrease of pH. Thus, low $K_{NH}$ value may suggest that the aeration and agitation system at Gliwice WWTP strips the produced CO\(_2\) efficiently, precluding significant drop of alkalinity (Siegrist & Tschui 1992). The increase of $K_{O,H}$ is not contradictory to this notion, as air bubbles may efficiently strip gaseous compounds having, at the same time, low oxygen transfer efficiency. The parameters of ammonification rate ($k_{A}$) and maximum specific hydrolysis rate ($k_{H}$) were decreased from 3.0 to 1.8 m\(^{3}\)·(gCOD d\(^{-1}\)) and 0.08 to 0.03 gCOD·(gCOD d\(^{-1}\)), respectively. The decreased values of $k_{H}$ and $k_{A}$ allowed reducing the rate of hydrolysis and ammonification of organic nitrogen, and, consequently, led to increase of the TKN concentration in the effluent.

In order to verify the predictive power of the calibrated parameters simulations were run using a new set of influent data from different time periods (period 2 and period 3). The main condition of the calibrated model verification was to keep all the adjusted model parameters constant so that obtained results are comparable. The results of simulations of the quality of the secondarily treated wastewater are shown in Figure 2, respectively for the period (abbreviated to Per) 1, 2, and 3. The analysis of the obtained results allows conclusion that the model has limited predictive ability and emulates the behaviour of the real system with an acceptable accuracy only for specific variables. The simulation results of N-NH\(_4\) concentration and TKN concentration in the effluent matches the measured data sufficiently, while the other variables, in particular, COD, TSS, N-NO\(_3\) and TN (total nitrogen) deviate from the measured data. This follows from the fact that the input of the biokinetic model, which was the output of the primary clarifier model, despite a significant degree of compliance with the measured data, was burdened with some errors. The simulation results of
ASM1 strongly depend on the quality of input data, hence any errors or inaccuracies in the characteristics of the influent, will decrease its predictive capacity. The primary treatment is aimed primarily to reduce the concentration of the TSS and COD. The greatest discrepancies between the results of simulations and the real data were observed for these variables. These differences also affected the predictions of the model in terms of N-NO₃ and TN concentrations. Model predictions for the sludge handling operation were evaluated based on simulation results of the VSS concentration in the digesters and the amount of biogas produced during anaerobic digestion process (Figure 3). By comparing the simulation results and measurement data for the mixed sludge concentration it can be concluded that the model correctly reproduces the real system mass balance of the sludge.

The simulation results of methane fermentation process were evaluated on the basis of daily production of biogas. For the data from the investigated periods an acceptable match with the real data was obtained. It should also be noted that the used digestion model represents a substantial simplification of real processes, which does not cover all aspects of methane fermentation. However, it can successfully be used to predict the effectiveness of the process and determine the biogas production in different conditions of the process.

CONCLUSIONS

Based on the performed modelling and simulation study the following conclusions were derived:

- the available construction and operational data of the WWTP, however limited, bares sufficient information to model and simulate its performance with an acceptable accuracy;
• the obtained model is neither finite or complete, but it is a sound basis for its further upgrade, and in
the current state it may be used to predict the effluent quality and the efficiency of biogas
production;
• the predictive capacity and its complexity may be enhanced, provided more detailed data are avail-
able, e.g. tracer tests, determination of crucial kinetic and stoichiometric parameters, oxygen
profiles, which are particularly needed for dynamic simulations; the model enhancement may
tain inclusion of model which will describe the plant behaviour with increased accuracy, e.g.
the AS and digestion models used in this study may be substituted with ASM2d and ADM1
models; also the modelling and simulation of the processes occurring in the primary settler could
be improved by inclusion of so-called reactive clarifier, which enables to mimic areal-world clarifier
in terms of physical and biochemical behaviour (e.g. production of volatile fatty acids); the obtained
model can be a basis for dynamic simulations and the obtained set of calibrated model parameters
can be regarded as estimates for model calibration using dynamic data;
• the inclusion of the simple model for primary settling allows studying the effect of sludge retention
on the efficiency of denitrification and the amount of produced biogas;
• commercially available dedicated software, such as WEST® can be used as platform for plant-wide
modelling studies without modifying the models available in the software.

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