Mathematical Modelling of Wastewater Treatment Plant
of Žiar nad Hronom

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Abstract

The calibration of Activated Sludge Model No. 1 (ASM1) for operational mode of wastewater treatment plant (WWTP) in Žiar nad Hronom was performed. Simulation program of single sludge process (SSSP), based on the Monod type biochemical reaction kinetics was applied. Measurements of diurnal variation of wastewater flow and composition at the influent and effluent of biological stage of the WWTP were carried out. The experimental data were transformed according to structure and process components of the mathematical model. Pre-denitrification system was used to transform alternating biological treatment technology operated at the WWTP to computer scheme. The calibration of mathematical model involved operational the parameter values (solid retention time, recirculation ratio) and the values of biokinetic parameters. The residual sum squares between the experimental and calculated values of process components was used as an objective function. Availability of the calibrated model for description of dynamic behaviour of the biological stage of the WWTP follows from the work.

Keywords: Biological processes, calibration, denitrification, dynamic behaviour, mathematical modelling, Monod kinetics, nitrification, simulation program, wastewater

Introduction

Biological processes are widely used for the removal of organic, nitrogen and phosphorus impurities from wastewater. Main reason is the possibility of achieving high elimination efficiency of these pollutants from wastewater. There are usually also lower capital and operational costs in comparison to physical-chemical and/or chemical processes.
A wastewater represents raw material with high flow and composition variability to be treated in order to rich required quality for discharging into receiving water. The extension of biological processes from carbonaceous impurities removal also to nitrogen and/or phosphorous removal has increased complexity of wastewater treatment systems. WWTP configurations and their operation are more complex. In addition, more stringent effluent quality limits have to be satisfied. Thus, the system must be well designed and operated optimally in order to meet these effluent standards with reasonable operational costs. The vast boom in computers and mathematical modelling in last decades have brought new possibilities also in wastewater treatment processes design and plant operation. Dynamic simulation programs are applied mainly for process operation and intensification. The objective of the work is to present the results of the calibration of the ASM 1 model for description of dynamic behaviour of biological stage at the WWTP in Žiar nad Hronom.

Theory
Numerical models for activated sludge plants have been becoming more popular and are generally used as a powerful tool to increase the detailed knowledge of the process and system behaviour, for optimisation studies, for training and teaching, and for model based process control over the last decades (Spering et al., 2008). The state-of-the-art model for biological wastewater treatment processes is the ASM1 (Henze et al., 1995). There are 13 process components, 8 biochemical processes, and 19 biokinetic parameters included in the model. Basically, the Monod type reaction kinetics is applied to describe the transformation of process components through biochemical processes included in this concept. The example of the Monod type reaction rate for oxygen consumption by aerobic growth of heterotrophs and autotrophs can be expressed as follows:

$$r_O = -1 - \frac{Y_H}{Y_H} \mu_H \left( \frac{\rho(S_S)}{K_S + \rho(S_S)} \right) \left( \frac{\rho(S_O)}{K_{O,H} + \rho(S_O)} \right) \rho(X_{B,H}) - \frac{4.57 - Y_A}{Y_A} \mu_A \left( \frac{\rho(S_{NH})}{K_{NH} + \rho(S_{NH})} \right) \left( \frac{\rho(S_O)}{K_{O,A} + \rho(S_O)} \right) \rho(X_{B,A})$$  \hspace{1cm} (1)

heterotrophs

autotrophs
where $K_{NH}$ is ammonium saturation constant (mg dm$^{-3}$), $K_{O,A}$ is oxygen saturation constant for autotrophs (mg dm$^{-3}$), $K_{O,H}$ is oxygen saturation constant for heterotrophs (mg dm$^{-3}$), $r_O$ is oxygen consumption rate (mg dm$^{-3}$ d$^{-1}$), $K_S$ is readily biodegradable organics saturation constant (mg dm$^{-3}$), $S_{NH}$ is ammonium nitrogen concentration (mg dm$^{-3}$), $S_O$ is dissolved oxygen concentration (mg dm$^{-3}$), $S_S$ is readily biodegradable substrate (mg dm$^{-3}$), $X_{B,A}$ is concentration of autotrophic biomass (mg dm$^{-3}$), $X_{B,H}$ is concentration of heterotrophic biomass (mg dm$^{-3}$), $Y_A$ is yield coefficient of autotrophic biomass (-), $Y_H$ is yield coefficient of heterotrophic biomass (-), $\mu_A$ is maximum growth rate of autotrophic biomass (d$^{-1}$) and $\mu_H$ is maximum growth rate of heterotrophic biomass (d$^{-1}$). The kinetics and stoichiometry of the model is typically presented in matrix form, e.g. Henze et al. (1987).

Various simulation programs for both steady state and dynamic simulations of nitrification and denitrification processes have been developed. The SSSP (Bidstrub et al., 1987) based on the above mentioned ASM 1 was used for dynamic simulations presented in the following part of the work.

**Materials and Methods**

**WWTP of Žiar nad Hronom**

This WWTP consists of mechanical and biological stage with aerobic sludge stabilization. Combined sewer system is used for wastewater collection. Mechanical pre-treatment consists of screens and aerated grid tank. Alternating denitrification treatment technology has been designed for the biological stage. There are 4 parallel oxidation ditches with total volume 12 000 m$^3$. Combined mechanical and pneumatic aeration are applied in order to introduce sufficient amount of oxygen for aerobic biological processes. Internal recirculation ratio varies from 50 to 100. Circular secondary settling tanks are applied to separate activated sludge from effluent wastewater. The WWTP was designed for total pollution load of about 59 000 population equivalents (p.e.), from which organic load corresponding to about 19 000 p.e. originates from industry. Actual organic load during performed dynamic measurements corresponded to 34 900 p.e.

**Alternating denitrification**

This biological treatment technology is known as Bio-Denitro process. The technology represents a technological modification of pre-denitrification (Pedersen a Sinkjær, 1992).
basic BioDenipho process consists of two circular reactors (oxidation ditches), which are operated alternatively as oxic and anoxic reactor. The alternating cycle is divided into four phases (Fig. 1). In phase A the raw wastewater is introduced into anoxic reactor (Reactor 2). Denitrification is performed in this reactor utilising organic pollutants in wastewater. Simultaneous accumulation of ammonium nitrogen from wastewater occurs during this phase.

At the same time, the first reactor (Reactor 1) is operated in under aerobic conditions. Thus, nitrification process and accumulation of nitrite and nitrate nitrogen are carried out in the reactor. The effluent from this reactor contains low ammonium and nitrate nitrogen concentration and is discharged to secondary settling tanks. In phase B there are both reactors operated in aerobic condition. The raw wastewater is introduced into the first reactor during
this phase. During this phase is second reactor (in previous phase operated as anoxic) prepared for discharging treated wastewater in the following phase (phase C). In phase C is the first reactor operated as anoxic and the second on is operated as oxic. The raw wastewater is introduced in the first reactor. Wastewater is discharged from the second reactor during this phase. Oxic conditions are maintained in both reactors during phase D. The raw wastewater is introduced into second reactor. Treated wastewater is discharged also from second reactor in phase D. Stage C and D present practically mirror image of stages A and B (Pedersen a Sinkjær, 1992).

High operational flexibility with regard to maintaining of oxic and anoxic volumes is characteristic for this technology. Aeration is switched off during anoxic phases. Sedimentation of activated sludge in reactor is prevented by mechanical mixing during these phases. Standard BioDenipho technology is usually designed for 57 to 67 % of nitrification volume and 33 to 43 % denitrification volume. If there’s need for enhanced biological phosphorus removal, the anaerobic stage can be involved in front of the circulation aeration tanks.

Wastewater flow and composition

Experimental measurements of diurnal variation of wastewater flow and composition at the influent and effluent of biological stage during 24 hours were carried out. The experimental concentration data of organic and nitrogen pollutants were transformed according to the structure and balanced process components in the ASM1 model. There are four fractions of organic pollution involved in the (Henze et al., 1987):

\[
COD_{\text{influent}} = COD_{\text{hom}} = S_S + S_I + X_S + X_I
\]  

where \(S_S\) is readily biodegradable substrate, \(S_I\) is soluble inert organic matter, \(X_S\) is slowly biodegradable substrate, \(X_I\) is particulate inert organic matter and \(COD_{\text{hom}}\) is chemical oxygen demand of homogenized sample. According to Pedersen a Sinkjaera (1992) Eq. (2) can be rewritten as follows:

\[
X_I = COD_{\text{hom}} - COD_{\text{filtr}} - K_{\text{BOD}} \cdot BOD_{\text{hom}} + K_{\text{BOD}} \cdot BOD_{\text{filtr}}
\]  

\(K_{\text{BOD}}\) and \(BOD_{\text{filtr}}\) are empirical parameters of the model.
where $K_{BOD}$ is biological soluble fraction of organic substrate expressed as COD, $BOD_{hom}$ is $BOD_5$ (biochemical oxygen demand) of homogenized sample and $BOD_{filtr}$ is BOD$_5$ of filtrated sample through membrane filter. Pedersen a Sinkjær (1992) published for municipal wastewater $K_{BOD}$ value 1.52.

Modification of Eq. (3) leads to:

$$COD_{hom} = COD_{filtr} + K_{BOD} \cdot BOD_{hom} - K_{BOD} \cdot BOD_{filtr} + X_I = COD_{filtr} + K_{BOD} \cdot BOD_{hom} - S_S + X_I = S_I + X_I + K_{BOD} \cdot BOD_{hom}$$

(4)

For particulate inert organics fraction it follows from Eq. (3):

$$X_I = COD_{hom} - S_I - K_{BOD} \cdot BOD_{hom}$$

(5)

Te content of soluble inert organic matter can be assessed as follows (Pedersen a Sinkjaera, 1992):

$$S_I = COD_{filtr} - K_{BOD} \cdot BOD_{filtr}$$

(6)

where $COD_{filtr}$ is COD of membrane filtrate of wastewater sample.

Likewise, the readily biodegradable organic fraction in wastewater can be evaluated as follows:

$$S_S = K_{BOD} \cdot BOD_{filtr} = S_{SS} + S_{SR} = 0.75 \cdot K_{BOD} \cdot BOD_{filtr} + 0.25 \cdot K_{BOD} \cdot BOD_{filtr}$$

(7)

where $S_{SS}$ is slowly biodegradable soluble and $S_{SR}$ is readily biodegradable soluble substrate. Thus, the inert soluble fraction $S_I$ can be calculated:

$$S_I = COD_{filtr} - S_S$$

(8)

Combination of Eqs. (6) and (8) gives:

$$COD_{hom} = S_I + X_I + K_{BOD} \cdot BOD_{hom}$$

(9)
Modification of Eq. (2) yields the following relationship:

\[ \text{COD}_{\text{hom}} = S_I + X_I + S_S + X_S \]  \hspace{1cm} (10)

Combination of Eq. (9) and (10) leads to:

\[ S_S + X_S = K_{\text{BOD}} \cdot \text{BOD}_{\text{hom}} \]  \hspace{1cm} (11)

\[ X_S = K_{\text{BOD}} \cdot \text{BOD}_{\text{hom}} - S_S \]  \hspace{1cm} (12)

Nitrogen pollutants content in wastewater when nitrites and nitrates are negligible can be evaluated as follows:

\[ N_{\text{tot}} = S_{\text{NH}} + S_{\text{ND}} + X_{\text{ND}} \]  \hspace{1cm} (13)

Where \( N_{\text{tot}} \) is total organic nitrogen, \( S_{\text{NH}} \) is ammonium nitrogen, \( S_{\text{ND}} \) is soluble organic nitrogen and \( X_{\text{ND}} \) is particulate organic nitrogen.

The following terms can be obtained for organic nitrogen fractions in wastewater when considering relationships involved in the database of SSSP simulation program:

\[ S_{\text{ND}} = 0.433 (N_{\text{tot}} - S_{\text{NH}}) \]  \hspace{1cm} (14)

\[ X_{\text{ND}} = 0.567 (N_{\text{tot}} - S_{\text{NH}}) \]  \hspace{1cm} (15)

Transformation of the WWTP layout into computer scheme

From the results of design calculations follows for pre-denitrification system total oxic volume 10 200 m\(^3\) and anoxic volume 1 500 m\(^3\). The designed total oxic volume for simultaneous denitrification is the same. The required anoxic volume is 2 600 m\(^3\) for this system. Thus, operational value of anoxic volume is better approximated with calculated denitrification volume for simultaneous denitrification. However, the whole bioreactor
volume by simultaneous activated sludge process exceeds the total volume of existing biological stage. Thus, pre-denitrification system was selected to approximate and transform of alternating denitrification technology into computer scheme.

**Results and Discussion**

The value of soluble inert COD content in the wastewater ($S_I$) was obtained experimentally. The sample of mixed liquor suspended solids withdrawn from the WWTP in Žiar nad Hronom was aerated in a batch system. COD content was analysed in filtered samples which were taken from the system at selected time periods. The results of the kinetic test are summarised in Table 1.

<table>
<thead>
<tr>
<th>t [h]</th>
<th>0</th>
<th>1.0</th>
<th>2.0</th>
<th>3.0</th>
<th>4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>COD [mg.l$^{-1}$]</td>
<td>65.8</td>
<td>53.9</td>
<td>47.9</td>
<td>47.9</td>
<td>47.9</td>
</tr>
</tbody>
</table>

Experimental value 47.9 mg.l$^{-1}$ for soluble inert COD ($S_I$) results from the batch test. The value of endogenous respiration rate 11.3 mg.g$^{-1}$.h$^{-1}$ (related to organic content of activated sludge) follows from respirometric measurements carried out with activated sludge sample taken from the WWTP. Experimental and calculated values of respiration rate at various concentration values of acetate are given in Table 2.

<table>
<thead>
<tr>
<th>$S$ [mg.l$^{-1}$]</th>
<th>0.96</th>
<th>1.91</th>
<th>3.83</th>
<th>4.78</th>
<th>5.74</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r_{X,exp}$ [mg.g$^{-1}.h^{-1}$]</td>
<td>15.5</td>
<td>24.9</td>
<td>23.5</td>
<td>28.7</td>
<td>82.5</td>
</tr>
<tr>
<td>$r_{X,calc}$ [mg.g$^{-1}.h^{-1}$]</td>
<td>12.9</td>
<td>23.6</td>
<td>40.8</td>
<td>47.7</td>
<td>53.7</td>
</tr>
</tbody>
</table>

The values of Monod equation parameters ($K_S = 10.0$ mg.l$^{-1}$ and $r_{X,max} = 147.3$ mg.g$^{-1}.h^{-1}$) were evaluated using grid search optimisation method. Corresponded values of respirometric rate $r_{X,calc}$ calculated using the above parameter values are also summarised in Table 2. Experimental values obtained during nitrification batch test performed with activated sludge sampled from the WWTP are given in Table 3.
The average value of ammonium nitrogen removal is 2.9 mg.g\(^{-1}\).h\(^{-1}\). The average value of specific rate of nitrite/nitrate nitrogen increase is 2.3 mg.g\(^{-1}\).h\(^{-1}\). Very low nitrification activity of activated sludge follows from nitrification batch tests when comparing with the literature data, e.g. 3 to 15 mg.g\(^{-1}\).h\(^{-1}\) (Chudoba et al., 1991).

### Table 3. Results of nitrification test

<table>
<thead>
<tr>
<th>t [h]</th>
<th>N-NH(_4) [mg.l(^{-1})]</th>
<th>N-NO(_3) [mg.l(^{-1})]</th>
<th>N-NO(_2) [mg.l(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>21.8</td>
<td>57.4</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>14.96</td>
<td>62.9</td>
<td>0.5</td>
</tr>
<tr>
<td>2</td>
<td>14.79</td>
<td>63.1</td>
<td>1.5</td>
</tr>
<tr>
<td>3</td>
<td>12.15</td>
<td>65.4</td>
<td>2.0</td>
</tr>
<tr>
<td>4</td>
<td>3.67</td>
<td>72.3</td>
<td>2.1</td>
</tr>
<tr>
<td>5</td>
<td>1.58</td>
<td>77.2</td>
<td>1.1</td>
</tr>
<tr>
<td>6</td>
<td>1.44</td>
<td>78.1</td>
<td>0.1</td>
</tr>
<tr>
<td>23</td>
<td>1.0</td>
<td>78.2</td>
<td>0</td>
</tr>
<tr>
<td>24</td>
<td>0</td>
<td>78.1</td>
<td>0</td>
</tr>
</tbody>
</table>

The calibration of the ASM 1 included examination of effect of operational parameter values (solid retention time (SRT), internal recirculation and recycle) and biokinetic parameter values on prediction of effluent wastewater pollution. The calibration was carried out with the aim to achieve minimum difference between experimental and calculated concentration values of effluent wastewater pollution. Effluent standard values given by the Slovak Governmental Regulation (2005) were used to evaluate the quality of effluent pollutants predictions by the model. The concentration values for individual pollutants in daily composite samples were calculated from the pollution loads as a flow-weighted (Q) average; for example, the concentration value of ammonium nitrogen in 24 hours composite sample was calculated as follows (Derco and Kovács, 2002):

\[
(N - NH_4)_{24-h} = \frac{\int_{t=0}^{24} Q(t) \cdot \rho(N - NH_4,t) \, dt}{\int_{t=0}^{24} Q(t) \, dt}
\]

Maximal values of N\(_{\text{tot}}\) were determined from N-NH\(_4\), N-NO\(_3\) and N\(_{\text{org}}\) in the effluent, i.e. maximal value for:
\[ \Sigma (N-NH_4 + N-NO_3 + N_{org}) = f(t) \] (17)

The time dependencies of ammonium nitrogen and nitrate/nitrite nitrogen concentration values for various values of return sludge recirculation ratio \( R_{rs} \) are presented in Fig. 2 and 3.

Fig. 2. Time courses of experimental (●) and calculated concentration values of N-NH\(_4\) (\(S_{NH}\)) in effluent for different values of \( R_{rs} \), ○ - 1.1; Δ - 0.9; * - 0.8; ◆ - 0.7.

Fig. 3. Time courses of experimental (●) and calculated concentration values of N-NO\(_2\) and N-NO\(_3\) in effluent for different values of \( R_{rs} \), ○ - 1.1; Δ - 0.9; * - 0.8; ◆ - 0.7.
Dynamic simulations were performed for SRT = 20 d and internal recirculation $R_{\text{rec}} = 0$ as the results of previous calibration.

Corresponded concentration values for ammonium nitrogen in 24-h composite samples as well as concentration values of oxic forms of nitrogen (nitrate and nitrite nitrogen) in 24-h composite samples are given in Table 4. The best correlation of the experimental data of ammonium nitrogen and oxic forms of nitrogen provides dynamic simulation performed with return sludge recirculation ratio $R_{\text{rs}} = 0.7$ (operational value was 1.1).

Table 4. Measured and calculated concentration values of nitrogen pollution in composite samples (SRT = 20 d, $Q = 8\, 210\, \text{m}^3\cdot\text{h}^{-1}$, $Q_{\text{rec}} = 0\, \text{m}^3\cdot\text{h}^{-1}$).

<table>
<thead>
<tr>
<th>$R_{\text{rs}}$</th>
<th>N-NH$_4$, 24-h [mg.l$^{-1}$]</th>
<th>N-NO, 24-h [mg.l$^{-1}$]</th>
<th>N$_{\text{inorg.}}$, 24-h [mg.l$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>1.40</td>
<td>7.40</td>
<td>8.80</td>
</tr>
<tr>
<td>0.9</td>
<td>1.37</td>
<td>7.02</td>
<td>8.39</td>
</tr>
<tr>
<td>0.8</td>
<td>1.37</td>
<td>8.36</td>
<td>9.73</td>
</tr>
<tr>
<td>0.7</td>
<td>1.36</td>
<td>8.76</td>
<td>10.12</td>
</tr>
<tr>
<td>0.6</td>
<td>1.34</td>
<td>9.22</td>
<td>10.56</td>
</tr>
<tr>
<td>0.5</td>
<td>1.32</td>
<td>9.73</td>
<td>11.05</td>
</tr>
<tr>
<td>0.4</td>
<td>1.32</td>
<td>10.31</td>
<td>11.63</td>
</tr>
<tr>
<td>exp.</td>
<td>0.53</td>
<td>8.08</td>
<td>8.61</td>
</tr>
</tbody>
</table>

Further decrease of return sludge flow is accompanied with highly negative effect on concentration values of oxic forms of nitrogen in comparison with positive effect on concentration value of ammonium nitrogen. Consequently, the content of total inorganic nitrogen ($N_{\text{inorg.}}$) in composite samples increased.

From the results of the ASM 1 model calibration for operation mode at WWTP in Žiar nad Hronom it follows that alternating denitrification technology can be approximated in computer scheme with acceptable quality by pre-denitrification system with zero internal recirculation and return sludge recirculation ratio $R_{\text{rs}} = 0.7$.

**Conclusion**

The ASM 1 model was calibrated for operational mode at the WWTP in Žiar nad Hronom. The SSSP simulation program was used. The measurements of diurnal variation of wastewater composition at influent and effluent of the biological stage were carried out. Significant organic shock load was observed during measurements.
The alternating denitrification system can be approximated by pre-denitrification system when transforming into computer scheme. The best fit between the experimental and predicted values of ammonium nitrogen and nitrite/nitrate nitrogen was achieved by dynamic simulation performed with return sludge recirculation ratio 0.7. From the results of the calibration it follows that the mathematical model describes the processes in alternating denitrification biological treatment system with sufficient accuracy from practical point of view although organic shock load occurred during measurements. It can be concluded that ASM 1 represents powerful and perspective tool for biological wastewater treatment processes operation. The model enables to predict the responses of the operated treatment system to changes in influent wastewater flow and composition as well as operational parameter values.

Acknowledgment

The authors wish to acknowledge the financial support from the Slovak Grant Agency for chemical and chemical-technological science (Grant No 1/0866/08) for this work.

References

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