# Utilization of Simulation Programs for Design of Biological Units for Nitrogen Removal

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The procedure of the utilization of dynamic simulation programs for design and upgrading of biological processes of nitrogen removal is presented. An upgrading of nitrification reactor to predenitrification system is illustrated. Design calculations were performed according to steady-state design practice. An optimization procedure for calculation of volume of denitrification reactor was developed. Minimizing of differences between required and calculated values of denitrified nitrogen is the merit of the applied method. Dynamic simulations were used for optimization of the dimensions of nitrification and denitrification reactors with regard to effluent standard values and fluctuations of wastewater flow and composition. A method for evaluation of dynamic simulation of results with respect to dynamic nature of wastewater effluent standards is suggested.

The Slovak Government Decree No. 242 [1] has established new effluent standards for wastewater discharge also for ammonium nitrogen. Moderate values are valid for the period before the end of 2004 and more stringent effluent concentration values are determined for the next period.

An approximation of our legislation on wastewater discharge quality to the European legislation has initiated an amendment of the above-mentioned Slovak Government Decree. The proposal of a new Slovak Government Decree [2] involves in addition to ammonium nitrogen effluent standards also total inorganic nitrogen standards.

According to the design practice wastewater treatment plants (WWTPs) are constructed with perspective at least 10 to 15 years from the beginning of operation. Thus it is assumed that new WWTPs have to be designed with regard to effluent standard values established for the period starting at the beginning of 2005.

The aim of the work is to verify a potential for upgrading biological wastewater treatment unit designed in accordance with actual legislation to biological unit which will satisfy perspective effluent standard values [2]. The upgrading of nitrification reactor to predenitrification system was selected as a study case. Utilization of dynamic simulations as a supporting tool for a steady-state design procedure is suggested. Dynamic simulations are applied to optimize biological unit dimensions with regard to transient behaviour of wastewater flow and composition.

# EXPERIMENTAL

The concentration values of wastewater components included in the database of the Simulation of Single Sludge Process (SSSP) program were applied as initial data for design and simulation calculations. These values are based on the concentrations of various constituents given by Metcalf & Eddy [3] for "typical" domestic wastewater, but they have been modified to be consistent with the constituents in the model and to account for the impact of primary sedimentation by *Bidstrup* and *Grady* [4]. This selection was encouraged by the similarities of wastewater flow and pollution diurnal patterns included in the database of the SSSP and diurnal values of  $\rho(\text{BOD}_5)$  and  $\rho(\text{COD})$ published by *Malý* [5] and *Chudoba et al.* [6].

The flow rate file included in the database of the SSSP gives an average daily flow of 1000 m<sup>3</sup> d<sup>-1</sup> and was scaled to give an average daily flow of about 9496 m<sup>3</sup> d<sup>-1</sup>. Plots of selected input files (flow rate Q, readily degradable substrate  $\rho(SS)$  and ammonium nitrogen  $\rho(N-NH_4^+)$ ) are presented in Fig. 1.

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Fig. 1. Feed flow rate and concentrations of readily biodegradable organics and ammonium nitrogen as a function of time. ■ Flow rate (Q), ▲ readily degradable substrate (SS), ● N—NH<sup>+</sup><sub>4</sub>.

Design calculations were performed using the following input data

 $\begin{array}{ll} Q = 9496 \ \mathrm{m^3 \ d^{-1}} & \rho(\mathrm{BOD}_5) = 167 \ \mathrm{mg \ dm^{-3}} \\ \rho(\mathrm{N--NH}_4^+) = 25 \ \mathrm{mg \ dm^{-3}} & \rho(\mathrm{N_{org}}) = 15 \ \mathrm{mg \ dm^{-3}} \\ \rho(\mathrm{X}_0) = 104 \ \mathrm{mg \ dm^{-3}} & \theta = 10 \ \mathrm{^{\circ}C} \\ \mathrm{p.e.} = 26 \ 431 & \rho(\mathrm{X}) = 2.5 \ \mathrm{kg \ m^{-3}} \end{array}$ 

where  $\rho(BOD_5)$  is the concentration of biochemical oxygen demand, p.e. population equivalent (the organic biodegradable load having BOD<sub>5</sub> of 60 g of oxygen per day [7]),  $\rho(N_{org})$  is the concentration of soluble and particulate organic nitrogen,  $\rho(X_0)$  concentration of solids in wastewater,  $\rho(X)$  activated sludge concentration in the reactor, and  $\theta$  is temperature.

The values of  $\rho(BOD_5)$  and  $\rho(X_0)$  were approximated based on the similarity of flow-weighted average concentrations in database of SSSP and those published for moderate polluted wastewater by *Henze et al.* [8]. The aim was to obtain more or less identical input data for performing design calculations and steady-state simulations. The other design values were equal to those flow-weighted average concentrations of wastewater components included in the database of the SSSP.

Dynamic simulations were accomplished by applying biokinetic parameter values for  $\theta = 10$  °C adopted from [9]. Time dependences of variability factors (ratio of actual and average concentration values) for Q, readily degradable substrate (SS), ammonium nitrogen (NH), organic soluble nitrogen (SN), slowly degradable substrate (XS), and particulate inert organic matter (XI) are shown in Fig. 2.

#### Activated Sludge Design Procedure

Design calculations for steady-state conditions according to ATV-A 131 [10] were applied.

The required aerobic solid retention time  $(SRT_A)$ 



Fig. 2. Variability factors as a function of time. □ Flow rate (Q), ■ SS, NH, SN, XS, XI.

for nitrification is calculated as

$$SRT_A = SF/\mu_{max} 1.103^{(\theta-15)}$$
 (1)

where SF is safety factor and  $\mu_{\text{max}}$  is maximum growth rate of *Nitrosomonas* (0.47 d<sup>-1</sup> at 15 °C). The safety factor SF considers mainly the daily nitrogen load fluctuations but also to some extent fluctuations of the maximum growth rate and short-range temperature and pH fluctuations, respectively [11].

Specific production of sludge (SPS) was calculated by the formula [12]

$$SPS = 0.6 \left( \frac{\rho(X_0)}{\rho(BOD_5)} + 1 \right) - \frac{0.432f}{\frac{1}{SRT_A} + 0.08f} \quad (2)$$

where f is the temperature correlation  $(f = 1.072^{(\theta - 15)})$ .

Volume  $(m^3)$  of aerobic (nitrification) reactor can be obtained as follows

$$V_{\rm N} = \frac{\rho({\rm BOD}_5) \cdot {\rm SPS} \cdot {\rm SRT}_{\rm A}}{\rho({\rm X})}$$
(3)

The total solid retention time (SRT) for the nitrification-denitrification system is calculated as

$$SRT = SRT_A / (1 - V_D / V_T)$$
(4)

where  $V_{\rm D}/V_{\rm T} = \beta$  is denitrification (anoxic) fraction of the total tank volume  $V_{\rm T}$  (m<sup>3</sup>) and  $V_{\rm D}$  is volume of denitrification reactor (m<sup>3</sup>).

The value of anoxic fraction  $\beta$  of the total reactor volume was obtained by the grid search optimization procedure. The difference between nitrogen concentration value to be denitrified and calculated actual effluent value of nitrogen was applied as the minimization function. Organic nitrogen, ammonium nitrogen, assimilated ammonium nitrogen, and nitrate nitrogen forms were balanced. The amount of assimilated nitrogen  $\rho(N_{asim}) \text{ (mg dm}^{-3})$  was calculated by the formula resulted for the design temperature  $\theta = 10 \,^{\circ}\text{C}$  by mathematical handling of graphical dependences for  $\rho(N_{asim})$  presented in [13]

$$\rho(N_{asim}) = (81.9179 - 15.7351 \ln SRT)\rho(BOD_5) \cdot 10^{-3}$$
(5)

The value of SRT was calculated by the equation as follows

$$SRT = \frac{1}{0.6 \frac{F}{\rho(BOD_5)}} (\rho(BOD_5) - \rho(X_0)) - 0.072\rho(X_a)f$$
(6)

where F/M is the food-microorganisms ratio, *i.e.* organic load of activated sludge (kg kg<sup>-1</sup> d<sup>-1</sup> BOD<sub>5</sub>/X) and  $\rho(X_a)$  is the concentration of active sludge.

The concentration of active sludge was calculated by the following equation [13]

$$\rho(\mathbf{X}_{a}) = 0.555 + 4.167 \left( 1.0 + \rho(\mathbf{X}_{0}) / \rho(\mathrm{BOD}_{5}) \frac{\mathrm{F}}{\mathrm{M}} / f \right) - \left( \left( 0.555 + 4.167 (1.0 + \rho(\mathbf{X}_{0}) / \rho(\mathrm{BOD}_{5})) \frac{\mathrm{F}}{\mathrm{M}} / f \right)^{2} - 8.3 \frac{\mathrm{F}}{\mathrm{M}} / f \right)^{-2}$$
(7)

Total recycle ratio  $(R_{\rm T})$  was obtained from the formula [12]

$$R_{\rm T} = E_{\rm D} / (100 - E_{\rm D})$$
 (8)

where  $E_{\rm D}$  is the efficiency of denitrification (%).

Recycle ratio of return activated sludge  $(R_{\rm RS})$  was calculated as follows [12]

$$R_{\rm RS} = \rho(\mathbf{X}) / (\rho(\mathbf{X}_{\rm RS}) - \rho(\mathbf{X})) \tag{9}$$

Concentration value of return activated sludge  $\rho(X_{RS})$  was obtained from the expression [12]

$$\rho(\mathbf{X}_{\rm RS}) = 1000/\rm{SVI} \tag{10}$$

where SVI is sludge volume index ( $\text{cm}^3 \text{ dm}^{-3}$ ).

# Simulation Program

The state-of-the-art model for biological wastewater treatment processes is the Activated Sludge Model No. 1 [9, 14]. This model allows to simulate carbonaceous pollutants removal, nitrification and denitrification processes. 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

I

v

t  $\mathbf{S}$  $\mathbf{S}$ 

h t С

10].

$$\begin{aligned} \mathbf{Y}_{\mathrm{O}} &= -\frac{1-Y_{\mathrm{H}}}{Y_{\mathrm{H}}} \mu_{\mathrm{H}} \left( \frac{\rho(\mathrm{S}_{\mathrm{S}})}{K_{\mathrm{S}} + \rho(\mathrm{S}_{\mathrm{S}})} \right) \cdot \\ &\cdot \left( \frac{\rho(\mathrm{S}_{\mathrm{O}})}{K_{\mathrm{O},\mathrm{H}} + \rho(\mathrm{S}_{\mathrm{O}})} \right) \rho(X_{\mathrm{B},\mathrm{H}}) - \\ &\text{heterotrophs} \\ &- \frac{4.57 - Y_{\mathrm{A}}}{Y_{\mathrm{A}}} \mu_{\mathrm{A}} \left( \frac{\rho(\mathrm{S}_{\mathrm{NH}})}{K_{\mathrm{NH}} + \rho(\mathrm{S}_{\mathrm{NH}})} \right) \cdot \\ &\cdot \left( \frac{\rho(\mathrm{S}_{\mathrm{O}})}{K_{\mathrm{O},\mathrm{A}} + \rho(\mathrm{S}_{\mathrm{O}})} \right) \rho(X_{\mathrm{B},\mathrm{A}}) \end{aligned}$$
(11)

where 
$$K_{\rm NH}$$
 is ammonium saturation constant (mg dm<sup>-3</sup>),  $K_{\rm O,A}$  oxygen saturation constant for autotrophs (mg dm<sup>-3</sup>),  $K_{\rm O,H}$  oxygen saturation constant for heterotrophs (mg dm<sup>-3</sup>),  $r_{\rm O}$  oxygen consumption rate (mg dm<sup>-3</sup> d<sup>-1</sup>),  $K_{\rm S}$  readily biodegradable organics saturation constant (mg dm<sup>-3</sup>),  $S_{\rm NH}$  ammonium nitrogen concentration (mg dm<sup>-3</sup>),  $S_{\rm S}$  dissolved oxygen concentration (mg dm<sup>-3</sup>),  $S_{\rm S}$  readily biodegradable substrate (mg dm<sup>-3</sup>),  $X_{\rm B,A}$  concentration of autotrophic biomass (mg dm<sup>-3</sup>),  $X_{\rm B,H}$  concentration of heterotrophic biomass (mg dm<sup>-3</sup>),  $Y_A$  yield coefficient of autotrophic biomass (-),  $\mu_{\rm H}$  maximum growth rate of autotrophic biomass (d<sup>-1</sup>), and  $\mu_{\rm H}$  maximum growth rate of heterotrophic biomass (d<sup>-1</sup>). The kinetics and stoichiometry of the model is typically presented in matrix form, *e.g.* by *Henze et al.* [9.

autotrophs

Various simulation programs for both steady-state and dynamic simulations of nitrification and denitrification processes have been developed. One of the versions of simulation program based on the abovementioned Activated Sludge Model No. 1 is Simulation of Single Sludge Process (SSSP) [4]. This program was used for dynamic simulations presented in the following part of the work.

#### **RESULTS AND DISCUSSION**

## **Design of Nitrification Reactor**

According to effluent standards given by the Slovak Government Decree No. 242 [1] ammonium nitrogen standard in wastewater discharges for agglomerations of more than 25 000 p.e. and time level after the year 2005 is established as follows

2.5

4338

8.7

8.5

 Safety factor
 2.0
 2.1
 2.2
 2.3
 2.4

  $V_{\rm N}$  m<sup>3</sup>
 3623
 3779
 3934
 4087
 4238

7.0

12.2

 Table 1. Results of Design and Simulation Calculations for Nitrification Reactor

\*Concentration values which satisfy effluent standard values.

d

 ${
m mg}~{
m dm}^{-3}$ 

 $\mathrm{SRT}_{\mathrm{ox}}$ 

 $\rho(N-NH_4^+)$ 

8-h composite sample

Table 2.	Results of	Design and	Simulation	Calculations	$\mathbf{for}$	Pre-Denitrification System
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Parameter		1.5	1.6	1.7	1.8	1.85	1.9
$V_{ m N}$	$m^3$	2814	2980	3144	3305	3386	3465
$V_{\rm D}$	$m^3$	601	628	655	680	692	705
$V_{\mathrm{T}}$	$m^3$	3416	3608	3799	3980	4078	4170
$\Theta_{\rm X,T}$	d	6.5	6.9	7.3	7.8	8.0	8.1
β	-	0.176	0.174	0.172	0.171	0.170	0.169
$Q_{\mathrm{I}}$	${\rm m}^{3}~{\rm d}^{-1}$	7506	7664	7811	7950	8018	8083
$\rho(\mathrm{NNH}_{4}^{+})$	$ m mg~dm^{-3}$	18.9	16.0	13.3	11.2	9.4*	9.1
24-h composite sample							
$\rho(\mathrm{NNH}_{4}^{+})$	$ m mg~dm^{-3}$	24.9	22.1	$19.4^{*}$	16.3	15.6	15.1
maximum conc.							
$\rho(\text{TIN})$	$ m mg~dm^{-3}$	23.0	21.7	20.7	$19.9^{*}$	19.1	19.0
24-h composite sample							
$ ho(\mathrm{TIN})$	$ m mg~dm^{-3}$	$28.5^{*}$	27.0	25.7	24.2	23.8	23.6
maximum conc.							

7.3

11.3

7.7

10.3

8.0

9.7\*

8.3

9.1

 $\rho(\text{N---NH}_4^+) \le 10 \text{ mg dm}^{-3}$  (8-h composite sample)

Design calculations (eqns (1-3)) were realized by applying various values of safety factor SF. Calculated values of reactor volume and operational parameters  $(R_{\rm RS}, {\rm SRT}_{\rm ox})$  were applied as parameter values of process flow scheme for dynamic simulations performed with SSSP program. Results of design and simulation calculations for nitrification reactor for selected values of SF are summarized in Table 1. Calculated value of return sludge ratio  $R_{\rm RS}$  was 0.33.

It follows from Table 1 that a sufficient value of SF with regard to the above given effluent standard value for 8-h composite sample is equal to 2.3.

## **Pre-Denitrification System**

The proposal of amendment of the Slovak Government Decree No. 242 [2] involves the effluent standards for nitrogen pollutants in wastewater discharges for considered agglomeration (more than 25 000 p.e.) as follows

$\rho(N-NH_4^+) \le 10 \text{ mg dm}^{-3}$	(24-h composite sample)
$\rho(N-NH_4^+) \le 20 \text{ mg dm}^{-3}$	(maximum daily
	concentration value)
$ ho({ m TIN}) \le 20 \ { m mg} \ { m dm}^{-3}$	(24-h composite sample)
$ ho({ m TIN}) \le 30 \ { m mg} \ { m dm}^{-3}$	(maximum daily
	concentration value)

where  $\rho(\text{TIN})$  is the concentration of total inorganic nitrogen, *i.e.*  $\rho(\text{N}-\text{NH}_4^+) + \rho(\text{N}-\text{NO}_3^-)$ .



Fig. 3. Pre-denitrification-activated sludge process. 1. Influent wastewater, 2. recirculation, 3. effluent wastewater, 4. returned sludge, 5. anoxic volume, 6. aerobic volume, 7. sedimentation tank.

Pre-denitrification system (Fig. 3) was selected to upgrade the above designed nitrification reactor in order to remove nitrogen pollutants according to the proposed effluent standards.

The results of design and simulation calculations for pre-denitrification system obtained for selected values of SF are summarized in Table 2. Dynamic simulations were performed with the values of nitrification and denitrification volumes, SRT, return sludge and internal recycle ratio values obtained by steadystate design calculations for individual values of SF (eqns (4-10)).

Fig. 4 depicts the influence of SF value on reactor volumes for pre-denitrification system. The effect of SF value on ammonium nitrogen concentration in 8-h and 24-h composite samples, respectively, and its maximum value is shown in Fig. 5. Similarly, Fig. 6 presents the dependences of  $\rho(\text{TIN})$  in 24-h compos-



Fig. 4. Dependences of reactor volumes on safety factor value for pre-denitrification system.  $\bullet$   $V_{\rm N}$ ,  $\blacktriangle$   $V_{\rm D}$ ,  $\blacksquare$   $V_{\rm T}$ .



Fig. 5. Dependence of ammonium nitrogen concentration on safety factor values for pre-denitrification system.
Grab sample, ● 8-h composite sample, ▲ 24-h composite sample.

ite sample and maximum value of this variable on SF value. From Figs. 4 to 6 it is obvious that SF value influences significantly both, reactor volumes (dominantly nitrification reactor volume) and effluent wastewater quality. This makes reasonable an effort to optimize this value.

From Table 2 it can be seen that a sufficient value of SF with regard to the above given effluent standard values [2] is equal to 1.85. The total volume necessary to carry out nitrification and denitrification processes is  $4078 \text{ m}^3$ . Thus nitrification process designed



Fig. 6. Dependence of total inorganic nitrogen concentration on safety factor value for pre-denitrification system.■ Grab sample, ● 24-h composite sample.

for ammonium concentration in 8-h composite sample in accordance with effluent standard value given in [1] provides potential for upgrading of nitrification and denitrification system satisfying effluent standard values involved in the proposal of amendment of the actual legislation [1].

The concentration values for individual pollutants in composite samples were obtained by integrating time dependences of wastewater flow and the pollutant effluent concentration. For example, the concentration of ammonium nitrogen in 24-h composite sample was calculated as follows

$$\rho(\mathrm{N--NH}_{4}^{+}) - 24 \cdot \mathrm{h} = \frac{\int_{t=0}^{24} Q(t)\rho(\mathrm{N--NH}_{4}^{+}, t)\mathrm{d}t}{\int_{t=0}^{24} Q(t)\mathrm{d}t} \quad (12)$$

Numerical integration was applied to solve eqn (12). The 8-h time period with the highest values of ammonium mass effluent, *i.e.* corresponding to the highest values of the product  $Q(t) \rho(\text{N}-\text{NH}_4^+, t)$  was considered. The interval between 13.25 and 21.25 hours is representative for the applied SSSP database. Maximum values of  $\rho(\text{TIN})$  were obtained from additive dependences of  $\rho(\text{N}-\text{NH}_4^+)$  and  $\rho(\text{N}-\text{NO}_3^-)$  vs. time

$$\sum \left[\rho(\mathrm{N--NH}_4^+) + \rho(\mathrm{N--NO}_3^-)\right] = f(t) \qquad (13)$$

Time courses of effluent ammonium and nitrate nitrogen as results of dynamic simulations for predenitrification system using steady-state design parameter values obtained for SF equal to 1.85 are illustrated in Fig. 7. Corresponding value of  $\rho(\text{TIN})$  in



Fig. 7. Variation of effluent ammonium and nitrate nitrogen concentrations with time in pre-denitrification system; safety factor value 1.9.  $\blacksquare \rho(N-NH_4^+), \bullet \rho(N-NO_3^-)$ .

24-h composite sample is 19.1 mg dm<sup>-3</sup> and maximum value of  $\rho(\text{TIN})$  is 23.8 mg dm<sup>-3</sup>. The values of these variables for selected SF values are plotted in Fig. 6.

# CONCLUSION

The procedure of the utilization of dynamic simulations as supporting tool for design of activated sludge system was developed. The upgrading of nitrification reactor to pre-denitrification system was applied as the case study. The aim was to verify the potential of upgrading of designed activated sludge system according to actual legislation with regard to effluent standards involved in the proposal of amendment of this legislation.

Design calculations were performed according to ATV design practice. The optimization procedure for calculation of volume of denitrification reactor was developed. Minimizing of differences between required and calculated values of denitrified nitrogen is the merit of the applied method. Dynamic simulations were used for verification of steady-state design calculations with regard to transient behaviour of nitrification and denitrification processes.

The method for evaluation of dynamic simulation results with respect to dynamic nature of wastewater effluent standards was suggested. Qualified grab sample was approximated by maximum value during diurnal cycle. Concentration values in composite samples were obtained by numerical integration of time profiles of wastewater flow and respective pollutant.

From the results it follows that for the considered agglomeration of about 26 500 p.e. there is the potential for upgrading of nitrification process designed according to the valid legislation to system performing nitrification and denitrification processes in correspondence with the effluent standards involved in the proposal of amendment of the Government Decree.

The relevance of the results is limited by applied database for design calculations and dynamic simulations. On the other hand, the procedure of utilization of dynamic simulation as a supporting tool for steadystate design calculation and the evaluation of the results of dynamic simulations with regard to transient nature of effluent wastewater standards are valid in general.

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