Modelling and simulation of a nitrification biofilter for drinking water purification

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Abstract

For the purification of pure and microbiologically safe drinking water, different treatment steps are necessary. One of those steps is the removal of ammonium, which can, e.g. be accomplished through nitrification in a biofilter. In this study, a model for such a nitrifying biofilter was developed and the model was consequentially used for scenario analysis. A protocol developed for characterisation of wastewater was used to characterise the biofilter influent. A comparison between measured and simulated effluent ammonium, nitrate and oxygen concentrations revealed that the predicting qualities of the constructed model are excellent. As such, the model could be used for further scenario analysis based on model simulations.

By simulating the behaviour of the biofilter, it was shown that its capacity to treat unexpected ammonium peaks in the summer time is very limited. Further simulations with the model showed that extensive aeration is not essential for nitrification as sufficiently dissolved oxygen is present in the influent. Therefore the aeration can be reduced to such a level that mixing is ensured. A final set of simulations showed that prolonged ammonium loads can be dealt with by reducing the influent flow rate. The amount of reduction depends of the operating temperature and influent ammonium concentration. The presented simulations can be used by the operators to reduce operating costs and as a decision tool in the case of high ammonium influent concentrations.

Keywords: drinking water purification, model-based optimisation, biofilter, ammonium removal, nitrification

Nomenclature

ASM	activated sludge model
BOD	biological oxygen demand (mgBOD/ℓ)
C^{sat}_{O2}	oxygen saturation concentration (mgO_2/ℓ)
COD	chemical oxygen demand (mgCOD/ℓ)
DO	dissolved oxygen (mgO_2/ℓ)
E(t')	dimensionless hydraulic residence time
HRT	hydraulic residence time (d)
K_La	oxygen transfer coefficient
NH_4^+	ammonium (mgN/ℓ)
S_S	biodegradable and soluble COD (mgCOD/ℓ)
S_I	non-biodegradable and soluble COD (mgCOD/ℓ)
T	temperature (°C)
T_{ref}	reference temperature (°C)
TIC	Theil's inequality coefficient
X_S	biodegradable and particulate COD (mgCOD/ℓ)
X_I	non-biodegradable and particulate COD (mgCOD/ℓ)
t	time (d)
t'	dimensionless time
y_i	simulated data points
$y_{i,m}$	measured data points
ρ	process rate (mgCOD/ℓ·d)
θ	Arrhenius constant
ϕ	temperature correction factor for oxygen transfer coefficient

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Introduction

The purification of pure and microbiologically safe drinking water is essential for limiting public health hazards. In Flanders, the northern part of Belgium, more and more surface water instead of groundwater is being used for drinking water purification in order to preserve the groundwater level. Surface water that is pumped into the drinking water purification site is treated with a series of biological and chemical techniques to ensure that the standards of safe drinking water are met. Examples of such techniques are the removal of ammonium through (biological) nitrification, the removal of phosphates and suspended particles by a combination of flocculation and filtration, the removal of micro-pollutants by active carbon filtration and disinfection with potassium hypochlorite.

Nowadays the operation of drinking water purification sites is based on experience (Rietveld, 2005). Water quality is monitored to prove that guidelines are met and, sometimes, laboratory tests are performed to determine, e.g. the dosage of chemicals. All these data, however, are scarcely used to improve day-to-day operation. The use of dynamic mathematical models, in combination with on-line monitoring and real-time control, can help to improve this day-to-day operation. This will lead to a better and more stable water quality, a better use of installed infrastructure and lower purification costs (Rietveld, 2005). Although dynamic modelling has been used frequently in other areas of chemical and environmental engineering, it has, however, only recently been applied in drinking water process modelling (Rietveld, 2005; Van der Helm and Rietveld, 2002; Rittman and Stillwell, 2002). In wastewater treatment modelling, for example, numerous examples exist of modelling, simulation and optimisation studies of both laboratory-scale and full-scale systems (Dochain and Vanrolleghem, 2001; Franks, 1972). The need for further research and the development of case studies is therefore evident.

In the case study presented here, the technique of dynamic mathematical modelling was used as a tool for analysis and optimisation of a nitrifying biofilter because of the above-mentioned benefits. The biofilter is used to remove ammonium from surface water as a first step in the purification of drinking water. The aim of the study was twofold:

- To develop a model describing the processes occurring in the nitrifying biofilter
- To use the model for scenario analysis.

Several methods developed for modelling and simulation of wastewater treatment plants, such as influent characterisation (Roeleveld and Van Loosdrecht, 2001), were applied in this study.

Methods

Description of the drinking water purification site

The drinking water purification site of the Vlaamse Maatschappij voor Watervoorziening (VMW, www.vmw.be) in Harelbeke (Belgium) withdraws water from the Kortrijk-Bossuit Canal (Cromphout and Rogge, 2002). This canal is fed by the Schelde River, which is the most important river in Flanders. The Schelde River is heavily polluted by industrial and municipal wastewaters over its entire course, although river water quality has improved during the past years because of the installation of several industrial and municipal wastewater treatment plants. At the current capacity the installation can produce 20 000 m³ drinking water per day, although in the future this capacity will be increased to 25 000 m³ of drinking water per day.

The water from the Kortrijk-Bossuit Canal is treated in a series of steps. As a first step ammonium and phosphate are removed from the water through biological nitrification and phosphate precipitation and filtration. After this first step the water then enters Gavers Pond, which is used for water recreation, such as swimming. After a residence time of on average 6 months water from the pond is pumped back to the water purification site for further treatment. This treatment consists of sand filtration, active carbon filtration, pH correction and the addition of potassium hypochlorite. This further treatment aims at removing suspended solids, micro-pollutants and germs.

Further details on the water purification installation are presented by Cromphout and Rogge (2002).

Description of the nitrifying biofilters

Three identical nitrifying biofilters operating in parallel are used for the removal of ammonium from the canal water through nitrification (Cromphout, 1992). The aim of these biofilters is to reduce the influent ammonium concentration to an effluent concentration of between 0 and 1 mgN/ℓ. This is to ensure that only a limited amount of ammonium enters the pond, consequently limiting the environmental and health risks associated with too high ammonium concentrations. For example, ammonia is already toxic to aquatic organisms at concentrations as low as 0.03 $mgNH_3$-N/ℓ (Solbe and Surben, 1989).

The biofilters are filled with carrier material that has a specific surface area of 400 m²/m³. As the total volume occupied by the carrier material in the 3 biofilters is 43.56 m³, the total surface area available for biofilm growth is 17 424 m². In the biofilter the total water volume for nitrification is 14.52 m³.

The raw canal water is introduced at the bottom of the biofilters at an average influent flow rate of 19400 m³/d and exits at the top. The air that supplies the biofilter with oxygen necessary for nitrification is also introduced at the bottom. The airflow rate is on average 300 m³/h. Because of the introduction of water and air at the bottom of the reactor the filter bed is slightly expanded.

Mathematical modelling

For the description of the biological processes (carbon oxidation and nitrification) occurring in the biofilter the Activated Sludge Model No. 1 (ASM1, Henze et al., 2000) was used. The default values as given in the ASM1 report (Henze et al., 2000) were used as values for the stoichiometric and kinetic parameters, as no specific conditions such as inhibiting substances or low oxygen concentrations (Wyffels et al., 2004) occur that make alterations to the parameters necessary.

The standard ASM1 was further extended with the insertion of a temperature dependency of the kinetics, because the temperature in the biofilters varies considerably during the year as they are subjected to ambient conditions. This is illustrated in Fig. 1 where the temperature in the biofilters is depicted over a 1-year period (1 September 2003 to 31 August 2004). In the figure time 0 corresponds with 1 September 2003. By applying an Arrhenius type of equation , the temperature dependency is included in the model:

$$\rho(T) = \rho(T_{ref})\, e^{\theta(T - T_{ref})}$$

where:

ρ: process rate
T is the actual reactor temperature
T_{ref} is the reference temperature, which was 20°C in this study
θ is the Arrhenius constant

The Arrhenius constants were calculated as proposed by Henze et al. (2000) based on the values for the kinetic parameters determined at 10°C and 20°C.

In addition, the oxygen transfer coefficient (ASCE, 1992) and the oxygen saturation concentration (*Standard Methods,* 1992) were made dependent on the temperature:

$$C_{O_2}^{SAT} = 14.65 - 0.41T + 7.99.10^{-3}T^2 - 7.78.10^{-5}T^3$$

$$K_L a = K_L a(T_{ref})\phi^{(T_{ref} - T)}$$

where:

C^{sat}_{O2} is the oxygen saturation concetration
K_La is the oxygen transfer coefficient
ϕ the temperature correction factor for the oxygen transfer coefficient (ϕ=1.02)

For the description of the typical processes occurring in the biofilter, such as the diffusion of solubles in the biofilm and the attachment and detachment of particulates to the biofilm, the model of Rauch et al. (1999) was used. The model is an extension of the well-known half-order reaction concept that combines a zero-order kinetic dependency on substrate concentration with diffusion limitation. The major advantage of the model is the simple structure which leads to a reduction of the computational effort as compared to state-of-the-art mixed-culture biofilm models (Rauch et al., 1999).

All simulations were performed in the modelling and simulation environment WEST® (Vanhooren et al., 2003).

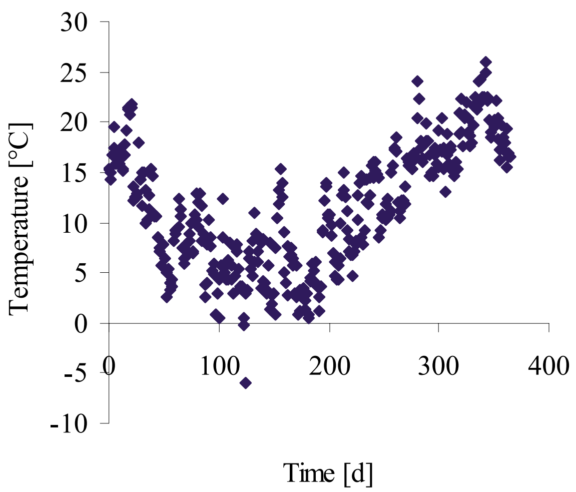


Figure 1
The temperature in the biofilter during a 1-year period

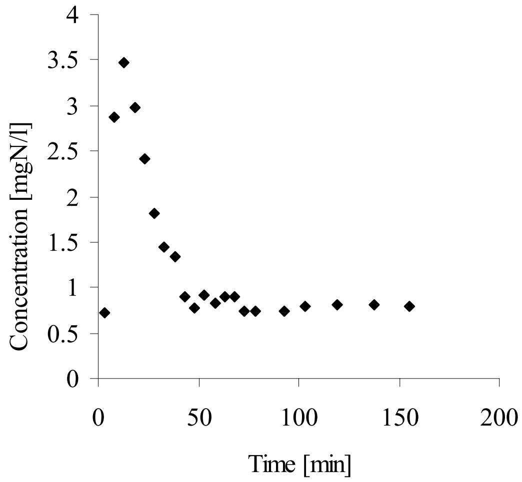


Figure 2
Measured effluent ammonium concentrations during the tracer test after injection of a pulse of 4 mgN/ℓ ammonium to the influent of one of biofilters at time 0

Hydraulic characterisation

The 3 biofilters operating in parallel are implemented in the WEST® software as one since all 3 are identical and fed with the same influent. In addition, a tracer test (Froment and Bishoff, 1990) performed on one of the biofilters was used to determine the hydraulic behaviour of the biofilter. With this tracer test the number of (perfectly mixed) tanks in series that correspond to the actual reactors hydraulic behaviour is determined.

For this tracer test a pulse of 4 mgN/ℓ ammonium was added to the influent of one of biofilters. Over a period of 2 h the effluent ammonium concentration was measured every 2.5 min. From the measured ammonium concentration $y_{NH4,m}(t)$ the dimensionless HRT distribution (E(t')) can be calculated:

$$E(t') = HRT\frac{y_{NH4,m}(t)}{\int_0^\infty y_{NH4,m}(t)dt}$$

where:

E(t'): the dimensionless HRT
$y_{NH4,m}(t)$: measured ammonium concentration
HRT: hydraulic residence time, which was 18 minutes at the time of the experiment
t: time [d]
t' = t/HRT [-] dimensionless time

The dimensionless HRT distribution can also be calculated theoretically as a function of the number of tanks in series (n) (Froment and Bishoff, 1990):

$$E(t') = \frac{n^n}{(n-1)!}t'^{n-1}e^{-nt'}$$

By comparing the experimentally obtained dimensionless HRT distribution curve to theoretical curves calculated for different values of *n* the optimal value of *n* can be determined.

Influent characterisation

A 1-year influent data-set was made available by the plant operators for modelling and simulation purposes. The data were collected over the period 1 September 2003 (denoted from now on as day 0) to 31 August 2004 (the latter is henceforth denoted as day 365) and contained daily or weekly measurements of influent flow rate, influent COD concentration, influent ammonium and nitrate concentration. Before these data can be used in the modelling study, a more thorough influent characterisation is however necessary as different COD fractions exist in the ASM1 (Henze et al., 2000) model. Indeed the total COD amount can be divided into biodegradable and soluble COD (S_S), non-biodegradable and soluble COD (S_I), biodegradable and particulate COD (X_S) and non-biodegradable and particulate COD (X_I). Furthermore, this influent characterisation is one of the dominant factors for the quality of model predictions (Roeleveld and Van Loosdrecht, 2001).

For the influent characterisation a physical-chemical method was applied (Roeleveld and Van Loosdrecht, 2001). However, instead of the proposed 0.1 µm filters 0.45 µm filters were used as according to Grady (1989) the term 'soluble' refers to material that passes through an 0.45 µm filter. These filters are used to distinguish between soluble and particulate material. All material that passes through the filter is considered as soluble, while all material that is retained is considered as particulate. Over a period of 3 months (September to November 2004) several grab samples of the influent and effluent were analysed. The total COD concentration, soluble COD concentration and BOD_{20} concentration were measured. Based on this analysis it could be determined how the total COD in the influent can be divided into the different COD fractions considered in the ASM1 (Henze et al., 2000) model.

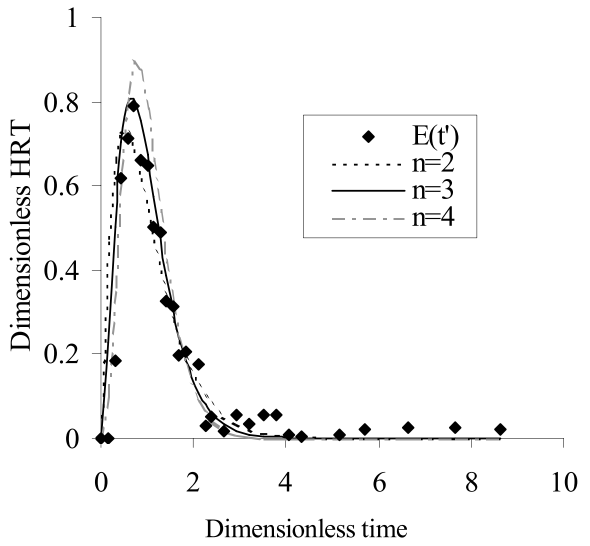
Chemical analyses

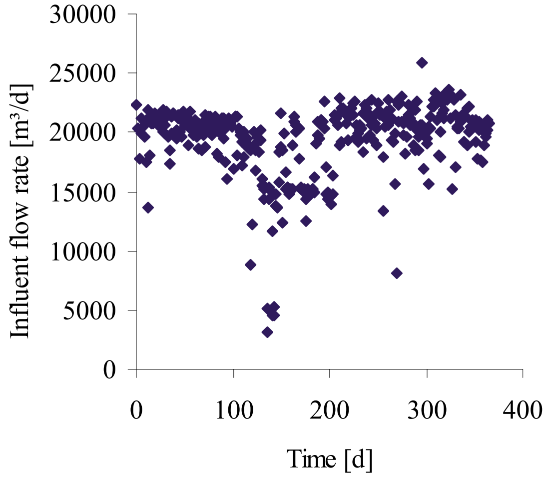
COD concentration, BOD_{20} concentration, ammonium concentration, nitrate concentration and oxygen concentration were all analysed according to standard methods (*Standard Methods*, 1992).

Results and discussion

Hydraulic characteristics

The results from the tracer test performed to determine the hydraulic characteristics of the biofilter are depicted in Fig. 2: the measured effluent ammonium concentrations are shown after injection of a pulse of 4 mgN/ℓ ammonium to the influent





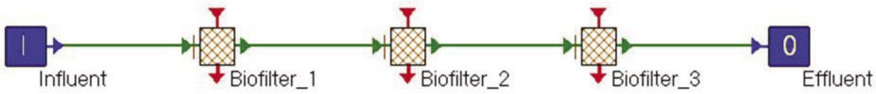


Figure 3 (top left)
Comparison of the experimentally obtained dimensionless HRT distribution curve to theoretical curves calculated for n equal to 2, 3 and 4

Figure 4 (left)
The schematic implementation of the biofilter in the WEST®

Figure 5 (top right)
Influent flow rate of the biofilter

of one of the biofilters at time 0.

In Fig. 3 the experimentally obtained dimensionless HRT distribution curve is compared to theoretical curves calculated for values of *n* equal to 2, 3 and 4. It can be seen that the theoretical curve corresponding with *n*=3 fits the experimental curves best.

From Fig. 3 it can be concluded that hydraulic behaviour of the biofilter can be represented by placing 3 tanks in series. Hence, the representation as given in Fig. 4 was used in WEST®.

Influent characteristics

In Fig. 5 the flow rate of the water pumped to the biofilter is given and Fig. 6 illustrates the concentration of ammonium, nitrate, DO and COD in the influent of the biofilter. In contrast to the influent flow rate, which is almost constant throughout the year (except when too high pollutions of the raw water necessitated flow reduction), the ammonium and nitrate influent concentrations have a highly season-dependent course. In summer time (from day 0 to day 50 and from day 200 to day 365) the temperature in the Kortrijk-Bossuit Canal, from which the water is withdrawn, is high enough to ensure nitrification. In winter time (from day 50 to day 200), however, temperatures are too low for full nitrification in the Kortrijk-Bossuit Canal. Hence, the influent ammonium concentration rises during winter. As such, it can be seen that the ammonium removal function of the biofilter is mainly necessary during the winter period. This cyclic behaviour of the ammonium influent concentration is repeated every year.

The influent characterisation revealed that approximately 85% of the total COD in the influent was soluble and inert. Another 5% of the total influent COD is particulate and inert. The remaining 10% is biodegradable and soluble. This means that about 90% of the total COD in the influent is not biodegradable. Indeed, the BOD_{20} measurements showed that very little biodegradable matter was present. As such this is not surprising as most of the biodegradable material will already be consumed by micro-organisms in the Kortrijk-Bossuit Canal.

As most of the COD is inert and the main purpose of the biofilters is to remove ammonium, the discussion of the simulation results will further be focused on the nitrification process.

Simulation results

In Figs. 7 and 8 the simulated effluent concentrations of ammonium, nitrate and DO are compared with measured values. From these figures it can be seen that the agreement is excellent. The oscillations in the ammonium and nitrate effluent concentrations around day 150 are due to short-term malfunctioning and/or shutdown of the installation. This is taken into account in the model as on a daily basis the influent flow rate is measured and used in the model. However, only weekly measurements of the effluent concentrations are used. Hence short-term (e.g. 6 h) disturbances will not be detected in the effluent measurements, but will be visible in the simulation results.

The measurement frequency of the DO concentration is rather low (once every month) and therefore the measured DO concentration seems more stable than the calculated DO concentration. The variation in DO concentration are mainly due to varying oxygen consumption and temperature conditions.

Moreover, the DO concentration around days 250-280 (15 mgO_2/ℓ) is rather high compared to the temperature conditions at that time (7-15°C). This is due to the fact that the influent at that time was supersaturated with oxygen at that time (see Fig. 6), even though the measurement frequency of the DO concentration is rather low.

The goodness-of-fit was further quantified by calculating Theil's inequality coefficient (TIC; Theil (1961)), which is expressed as follows:

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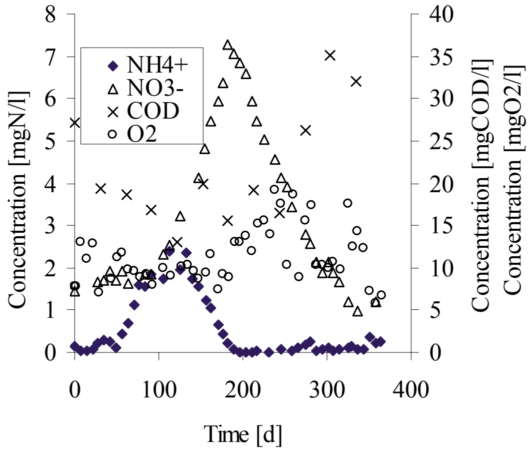

Figure 6
Concentration of ammonium, nitrate, dissolved oxygen and COD in the influent of the biofilter

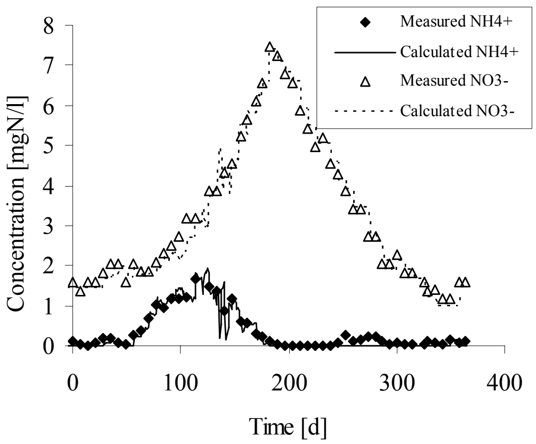

Figure 7
Comparison between measured and simulated effluent ammonium and nitrate concentrations

$$TIC = \frac{\sqrt{\sum_i \left(y_i - y_{m,i}\right)^2}}{\sqrt{\sum_i y_i^2} + \sqrt{\sum_i y_{m,i}^2}}$$

where:

y_i represents the simulated data points

$y_{i,m}$ representing the measured data points

A value of the TIC lower than 0.3 indicates a good agreement with measured data (Zhou, 1993).

The TIC was determined for both the winter time (days 50 to 200) as the complete experimental period (days 0 to 365), because the filter receives significant ammonium loads during winter time, while during summer almost no ammonium enters the biofilters.

For the effluent concentrations of ammonium, nitrate and DO during winter time a TIC of 0.14, 0.052 and 0.068 respectively was obtained. If the TIC was calculated for the 3 measurements combined as one, a value of 0.063 was obtained for the winter time values.

For the effluent concentrations of ammonium, nitrate and DO over the complete experimental period a TIC of 0.16, 0.053 and 0.149 respectively was obtained. If the TIC was calculated for the 3 measurements combined as one, a value of 0.12 was obtained.

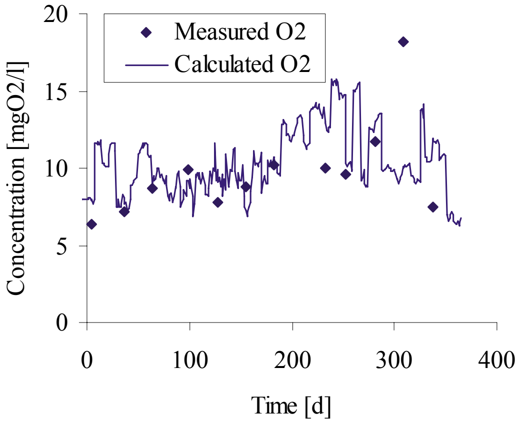

Figure 8
Comparison between measured and simulated effluent DO concentrations

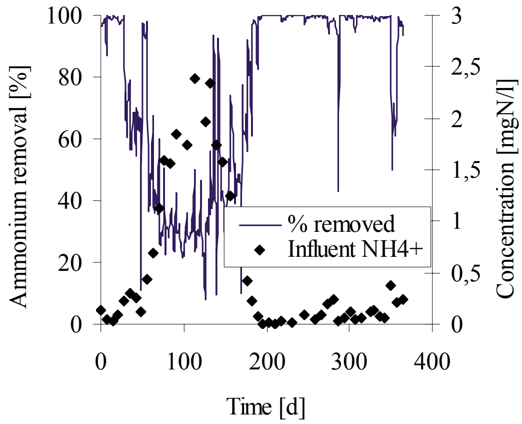

Figure 9
The amount of ammonium removed in the biofilters and the influent ammonium concentration

As such the biofilter model can be considered to describe the behaviour of the biofilter properly and thus this model can be used for further scenario analysis. This way potential bottlenecks and operational improvements can be demonstrated.

Biofilter performance

On the other hand it can be concluded from Figs. 7 and 8 that the performance of the biofilters is not very good. During wintertime (period from day 50 until day 200), when there is substantial ammonium in the influent, the amount of ammonium removed decreases to a minimum of 30%. This can be seen from Fig. 9. In this figure the amount of ammonium removed in the biofilters is given as a percentage. An indication of the influent ammonium concentration is also given.

In Fig. 10 the calculated thickness of the biofilm is shown in each of the 3 reactors that describe the hydraulics as represented in Fig. 4. Logically, the thickness of the biofilm decreases from biofilter 1 (the front of the biofilter) to biofilter 3 (the end of the biofilter) as the first reactor will deal with the highest influent concentrations. Also, the biofilm is significantly thicker during the winter period (from day 50 to day 200) compared to the summer period as there is growth of nitrifying organisms in the winter due to the presence of ammonium in the influent. This limited amount of nitrifying organisms and, consequentially, lower biofilm thickness during the summer period limits the capability

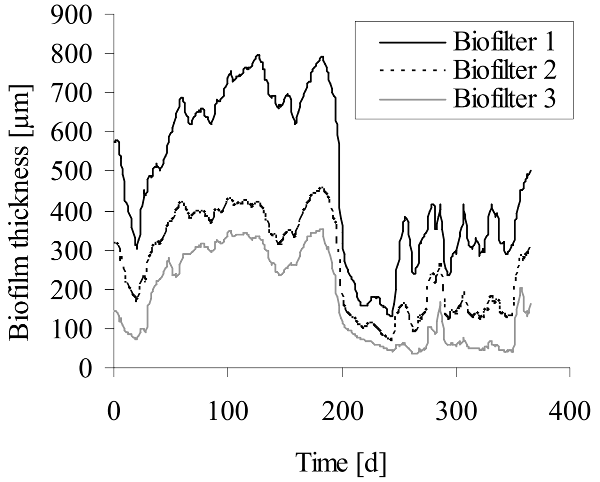

Figure 10
The calculated thickness of the biofilm in each of the 3 reactors represented in Fig. 4

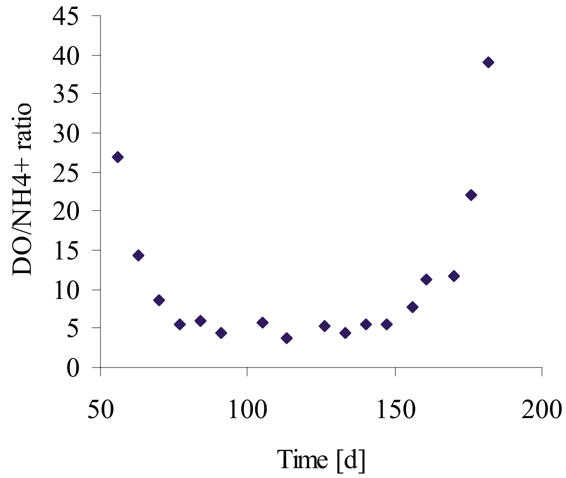

Figure 11
Ratio of influent DO to influent ammonium from day 50 to day 200

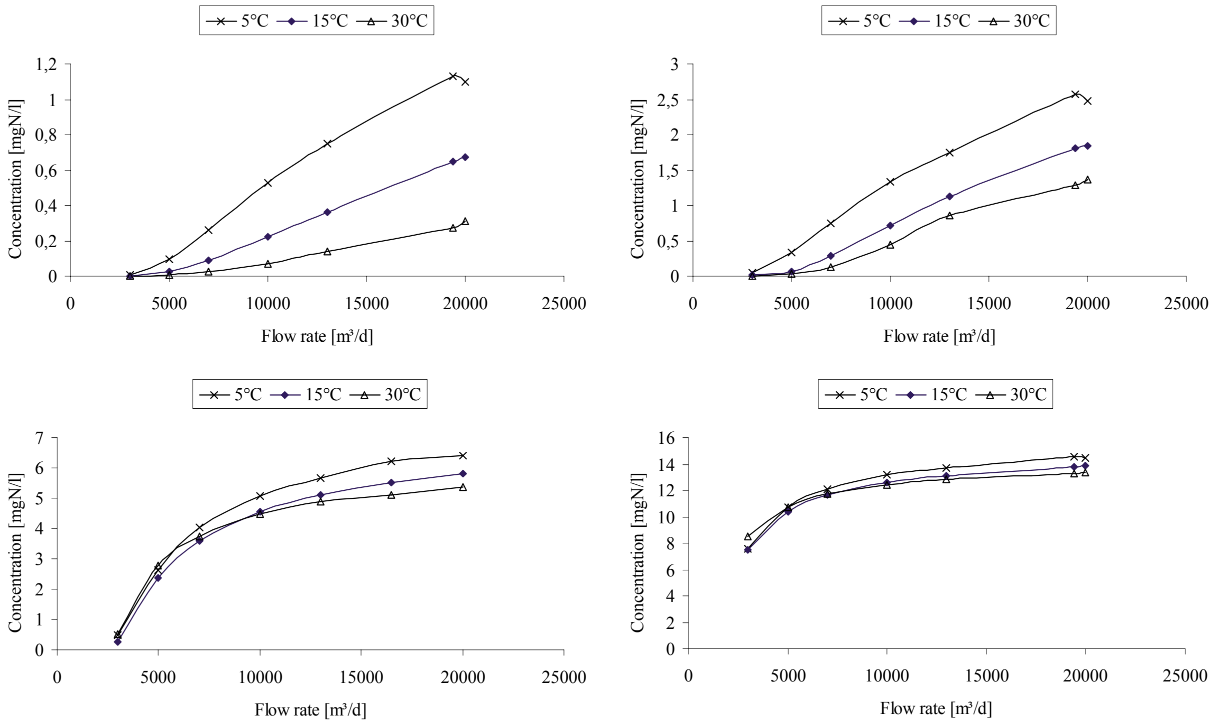

Figure 12
Effluent ammonium concentration resulting from an influent ammonium concentration of 2 mgN/ℓ (top left corner), 4 mgN/ℓ (top right corner), 8 mgN/ℓ (bottom left corner) and 16 mgN/ℓ (bottom left corner)

of the biofilter to remove sudden peaks in ammonium concentration that may occur.

Model-based optimisation and scenario analysis

First the effect of reducing the aeration of the biofilter was investigated. This was done because from a preliminary back-of-the-envelope calculation it became clear that the amount of oxygen present in the influent would be sufficient to oxidise the ammonium in the influent. This is illustrated in Fig. 11 where the ratio of influent DO to influent ammonium is depicted from day 50 to day 200. Outside this period the DO ammonium ratio is higher than 10, while during this period the ratio never drops below 3.8. This high ratio results from the fact that the canal water is vigorously mixed before entering the biofilter. At certain periods, the canal water is even supersaturated with oxygen. Hence, little or no aeration is necessary for complete nitrification as theoretically the amount of DO necessary to completely oxidise ammonium is 4.57 gO_2/gN (Henze et al., 1995). This preliminary calculation was confirmed by simulating the behaviour of the biofilter when aeration was turned off. For the simulated ammonium and nitrate concentrations in the effluent the same results were obtained as in the case depicted in Fig. 7 where there was aeration. As could be expected, however, the DO concentration was lower.

Because aeration is also used for mixing purposes it can

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be concluded that important savings in aeration costs can be accomplished if the aeration would be reduced to a level that still guarantees the mixing.

The effect of different ammonium influent concentrations (2, 4, 8, 16 mgN/ℓ), e.g. resulting from illegal and/or industrial discharges or agricultural runoff to the canal Kortrijk-Bossuit, was also investigated. These discharges are the main reason for a sudden or prolonged increased ammonium concentration in the rivers. Especially during the period that fertilisation of agricultural land is permitted in Flanders (15 February to 31 August) a risk of increased ammonium concentration exists. In order to have a strategy to deal with these increased concentrations the below discussed experiments were performed, keeping in mind that the biofilter is the only place where ammonium is removed in the drinking water purification process.

Simulations were performed at 3 different temperatures, 5, 15 and 30°C, corresponding with winter, average and summer conditions, respectively. In Fig. 12 the resulting effluent ammonium concentration as function of different influent flow rates is depicted. As can be expected the removal of ammonium is higher at higher temperatures because of the higher process rates. Of course sufficient biomass should be present in the biofilter, otherwise problems as discussed above are to be expected.

From this figure it also becomes clear that an increased influent ammonium concentration can be treated to a desired effluent concentration by lowering the influent flow rate. In case the influent ammonium concentration is too high, e.g. 16 mgN/ℓ, a complete stop of the influent flow might be necessary to avoid too high effluent concentrations.

Another approach would be to increase the amount of filter material in the reactor and by doing so increase the residence time. As such, lower effluent concentrations are to be expected.

Fig. 12 can be used by plant operators as a decision-making tool in case of too high influent ammonium concentrations. Hence, the mathematical trickling filter model offers the possibility to evaluate possible high-risk situations and their solutions. Testing these situations on the full-scale plant is not possible because the quality of the drinking water has to be ensured.

Conclusions and perspectives

A model for a biofilter used in the purification of drinking water was constructed and subsequently used for process simulations. To characterise the influent of the biofilter a calibration protocol developed for characterisation of wastewater was followed. This characterisation revealed that most of the influent COD was inert and further attention was therefore only paid to the nitrification process, as this is also the main purpose of the biofilter. Comparison between measured and simulated effluent ammonium, nitrate and oxygen concentrations revealed that the predictive ability of the constructed model was excellent. With the simulations it was also shown that the capacity of the biofilter to treat unexpected ammonium peaks in the summer time is very limited. Scenario analysis with the model showed that aeration is not essential for nitrification as sufficiently dissolved oxygen is present in the influent. Therefore the aeration can be reduced to such a level that mixing is ensured. Extra peak loads of ammonium can be dealt with by reducing the influent flow rate. The extent of the reduction is dependent on the operating temperature and influent ammonium concentration.

The simulation results presented in this work will be used by water purification plant operators as a decision-making tool in case of increased ammonium influent concentrations. Based on the simulation results it can be decided how much the influent flow rate should be decreased to ensure proper operation of the biofilters. Further, cost savings will be accomplished by reducing the air flow rate.

This study should be seen as a first step in a model-development and model-based optimisation project that aims at modelling the complete drinking water purification facility. In addition, the influence of the canal Kortrijk-Bossuit will be studied using dynamic models, as the canal water has a large effect on treatment performance and costs. As such, it will be possible to model the purification of drinking water 'from the river to the tap.'

Of course, the results of this study are not specific only for the water purification facility of the VMW in Harelbeke, but it is possible to use these results in other water purification facilities as well, both in Flanders and world-wide.

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