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Scenario analysis and statistical analysis of simulation results of operation of activated sludge waste water treatment plants

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ABSTRACT

Several studies, both theoretical and experimental, have already proven that mathematical modelling of wastewater treatment plants (WWTP) is an elegant and cost-effective tool to study and to optimise these treatment processes. In most cases, interpretation of the simulation results is done on ad hoc complex databases based on so-called expert knowledge. As such, the interpretation of the results becomes difficult. In this study, interpretation of the WWTP simulation results is aided by the means of principal component analysis (PCA). The main influencing factors were found to be the influent flow rate and load, and the settler performance in terms of the non-settleable fraction of the biomass. A PCA analysis indicated three principal components. The first principal component explained 37% of the total variance and contains most of the information on nitrogen removal. The second principal component (PC2) explains 20% of the total variance and can be considered as a measure of the secondary settler performance. The third principal component (PC3) explains 17% of the total variance and mostly contains information on the different flow rates in the WWTP (influent flow rate, nitrate recycle flow rate, sludge recycle flow rate and waste flow rate).

Keywords: Scenario analysis; Statistical evaluation; ASM1; Modelling and simulation; Principal components analysis

1. Introduction

Several studies, both theoretical and experimental, have already proven that mathematical modelling of wastewater treatment plants (WWTP) is an elegant and cost-effective tool to study and optimise these treatment processes [1]. Modelling offers the possibility to investigate certain engineering questions without time-consuming and expensive laboratory tests. In the last 30 years, relatively reliable dynamic simulation models for the activated sludge process, including biological N and/or P removal [2–4] have been developed. These models have been summarised in the activated sludge models series (ASM1, ASM2, ASM2d and ASM3, [4]). ASM models have been used and extended for specific case studies (e.g. greenhouse gas production). Especially, large scale treatment systems are almost routinely modelled for all sorts of applications. Choubert et al. [5], for example, evalu-

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ated two operating strategies of activated sludge systems to cope up with the increase in carbon and nitrogen loading rates, generally, observed on WWTP located in the winter resorts. Brdjanovic et al. [6] used a model for better understanding of full-scale biological phosphorus removal. Rousseau et al. [7] presented a review on design models for horizontal subsurface flow constructed treatment wetlands. Vandekerckhove et al. [8] used an ASM1-based model to assess different upgrade scenarios of a food industry WWTP, while Van Hulle and Vanrolleghem [9] used an extended ASM1 model to optimise the operation of a chemical industry WWTP. Fang et al. [10] used a dynamic model to simulate full-scale municipal WWTP behaviour under fluctuating conditions.

In most cases, interpretation of the simulation results is done ad hoc based on so called expert knowledge. However, the increase in computational capacity of the personal computer has led to an exponential increase in the number of performed simulations. This results in huge and complex data bases which are often difficult to interpret, and hence it becomes difficult to draw meaningful conclusions. Recently, the use of efficient statistical tools such as principal components analysis (PCA), multi-criteria decision analysis and uncertainty analysis to facilitate the interpretation of these large sets of simulation results was introduced [11–14].

The aim of this study is to demonstrate how PCA can be used to interpret simulated scenarios of the operation of a waste water treatment plant. PCA was used as it is useful for data reduction and to assess the continuity/overlap of clusters or clustering/similarities in the data [15]. The WWTP was designed based on general design rules [16] and was implemented in the modelling and simulation WEST® platform (www.mikebydhi.com) [17]. To our knowledge this is the first time that such a large WWTP simulation dataset is interpreted by PCA or any bother statistical tools. This in contrast to the measurement data [13,18–20]. As such, the main aim of the study was to statistically interpret the ASM-based simulation results when ad hoc interpretation is not possible anymore due to the large dataset. By combining both the simulation results and the statistical analysis, an insight in the operation of the WWTP can be obtained.

2. Materials and methods

2.1. WWTP design and model

A WWTP was designed based on the general design rules [16] and acts as an example WWTP. In future, other WWTP configurations could be investigated such as the ones provided by the Benchmark simulation model guidelines [21,22]. A pre-denitrification layout was used for COD and nitrogen removing WWTP. The volume of the anoxic reactor was chosen to be 1,500 m^3, while the volume of the aerobic reactor was chosen to be 3,000 m^3, which results in an aerobic/anoxic volume ratio of 2/1. Different kind of operational conditions were simulated (see below).

The WWTP was implemented in the modelling and simulation software WEST® (www.mikebydhi.com) [17]. Although the activated sludge reactors have a very large volume, they can still be considered as ideally mixed [9]. An ideal point settler with a non-settleable fraction of the biomass (f_{ns}) was considered as an appropriate model for the secondary settler, similar to the work of Van Hulle and Vanrolleghem [9]. The non-settleable fraction of the biomass (f_{ns}) reflects both the settling properties of the biomass and the operational performance of the settler. An insufficient residence time for example will lead to a higher f_{ns} value. The non-settleable fraction of the biomass (f_{ns}) was set at two different values: 0.1 and 0.5%.

The activated sludge processes (bacterial growth and decay) were described by the activated sludge model 1 (ASM1; [4]). Both COD and nitrogen removal are incorporated in this model. For the simulations, default parameter values were used as specified by Henze et al. [4]. Parameter uncertainty was not studied as this is the focus of other research (e.g. [11]). Also, this study wants to focus more on the interpretation of the modelling result and the translation of the modelling findings to practice.

In total five different influent concentrations were simulated: 125, 250, 500, 750 and 1,000 mg COD/l. COD fractionation, that is, the conversion of the influent COD concentration to the variables used in ASM1 was based on Goudeseune and Van Hulle [23]. The influent COD concentration was as such divided into a soluble, biodegradable fraction (S_S), a soluble non-biodegradable fraction (S_I), a particulate biodegradable fraction (X_S) and a particulate non-biodegradable fraction (X_I). This division is presented in Table 1. The nitrogen content was assumed to be 10% of the COD content, which is the ideal C/N ratio. Also, it was assumed that 90% of the nitrogen content was ammonium and the remaining 10% was assumed to be soluble organic nitrogen.

In order to mimic different design choices and as such different operational performances, simulations with three different hydraulic residence times (0, 5, 1 and 1, 5 days), three different oxygen set-points (2, 4 and 6 mg/l) were run. The oxygen set-points were chosen to have a wide range of possible oxygen concentrations and were controlled by adapting the K_La value of the aerobic reactor. As strict oxygen con-

Table 1
Classification of the influent COD concentration in the different fractions expressed as percentage of total influent COD concentration

Component	Fraction of the total influent COD concentration (%)
S_S	22
S_I	7
X_S	35.5
X_I	35.5

trol was implemented, the actual oxygen concentration did not vary significantly from the set-point. Two different reactor configurations (one and five tanks in series for both the aerobic and the anoxic reactor) were performed. In case, if five tanks in series were assumed, the volume of each tank was assumed to be 1/5 of the total tank volume. Also, three different activated sludge concentrations were used: 2,500, 4,000 and 6,000 mg/l. The activated sludge concentration was maintained in the reactors by controlling the waste flow rate. The nitrate recycle and the sludge

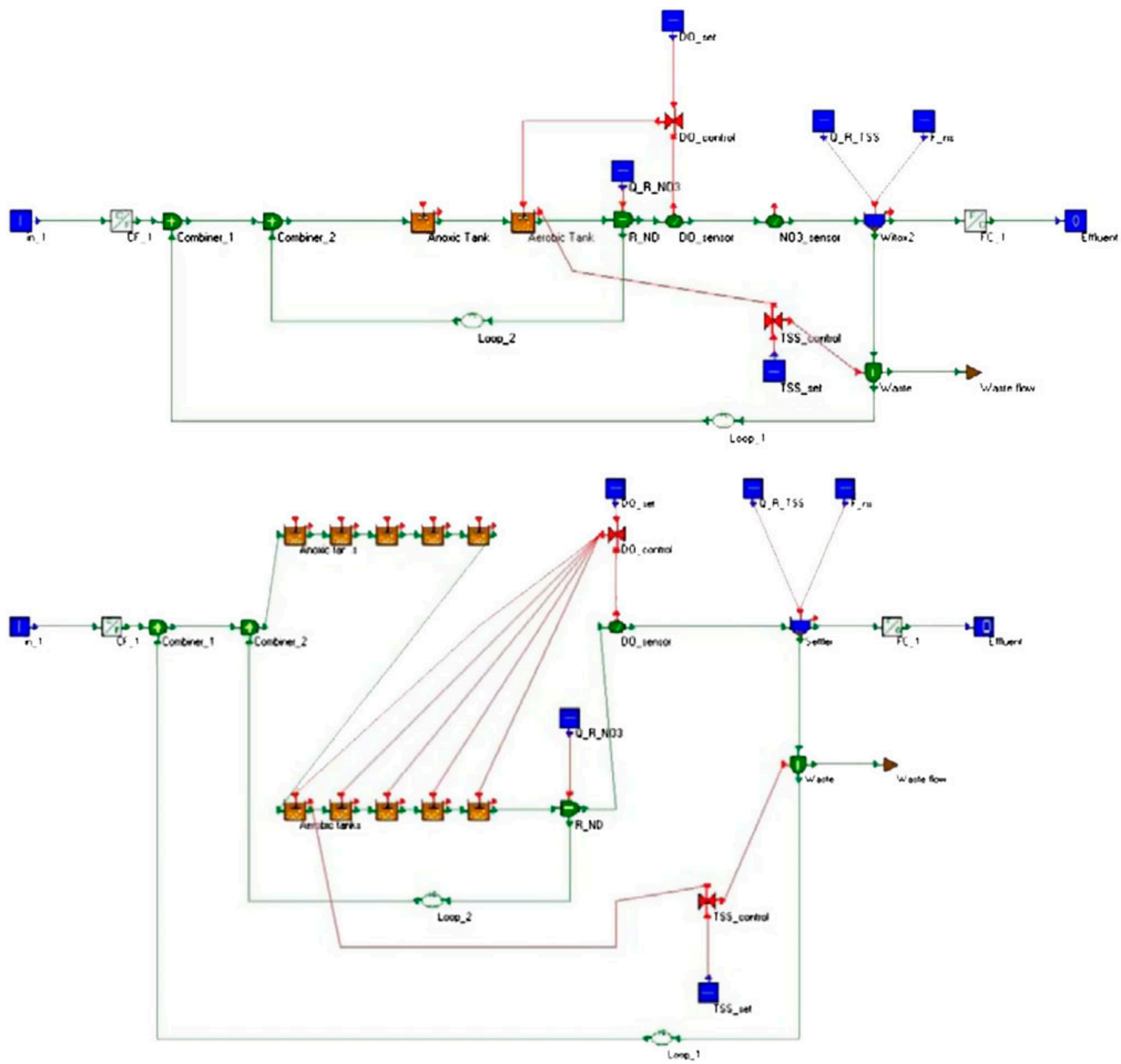

Fig. 1. The implementation of the studied WWTP in the modelling and simulation software WEST® (top: 1 reactor implementation; bottom: 10 reactors in series implementation).

Table 2
Summary of the scenario analysis in terms of percentage of discharge limit violations

Effluent value	Discharge limit	Percentage of violations (%)
Effluent COD	125 mgCOD/l	10
Effluent BOD	25 mgBOD/l	3
Effluent suspended solids	35 mg/l	35
Effluent total nitrogen	15 mgN/l	42

recycle flow rate were assumed to be a percentage of the influent flow rate. For the nitrate recycle 50, 100 and 200% of the influent flow rate was used, while for the sludge recycle flow rate 50, 100 and 300% of the influent flow rate was used.

This resulted in the following two implementations in WEST® (Fig. 1). All simulations (in total 4,860 scenario's obtained by combining the above mentioned design settings) were performed until steady state. The complete set of results in given as supplementary material and the main findings will be discussed in the results section.

Next to the effluent concentrations and the removal percentages, also the operational costs were calculated. The resulting effluent fines were calculated based on the formula imposed by the Flemish Environment Agency (www.vmm.be, www.heffingen.be).

$$H = N \times T$$

$$N = N1 + N2$$

$$N1 = \frac{Q}{180} \times \left(0.35 \times \frac{SS}{500} + 0.45 \times \frac{2 \times \mathrm{COD} + \mathrm{BOD}}{1,350}\right)$$

$$N2 = \frac{Q \times N}{10,000}$$

where H—effluent fines (€/y); T—effluent tariff (31,67 €); Q—flow rate (m^3/y); SS—effluent suspended solids concentration (mg/l); COD—effluent COD concentration (mg COD/l); BOD—effluent BOD concentration (mg BOD/l), assumed to be the sum of soluble, biodegradable COD and particulate, biodegradable COD and N—effluent nitrogen concentration (mg N/l).

The pumping energy (PE) was calculated based on the influent flow rate, the nitrate recycle flow rate, the sludge recycle flow rate and the waste flow rate by assuming a PE of 0.075 kWh/m^3 for the first three flow rates and a PE of 0.05 kWh/m^3 for the waste flow rate [24].

The mixing energy (ME) was calculated according to Fenu et al. [25], based on the value of 63.6 kWh/m^3/j. As the volume of the reactors was the same for every simulation, this ME was also the same for the different scenarios.

The aeration energy (AE) was calculated according to Nopens et al. [22] based on the oxygen transfer rate (OTR) and assuming a transfer efficiency of 1.8 kg O_2/kWh used.

$$AE = \frac{OTR}{1.8} = \frac{V \times K_l a \times S_O^{SAT}}{1,000 \times 1.8}$$

where V—volume of the aerobic reactor (1,500 m^3); $K_l a$—aeration rate (y^{-1}); S_O^{SAT}—oxygen saturation concentration (8 mgO_2/l).

The three types of energy discussed above are expressed in kWh/y. For conversion o euro/year an electricity cost of 0.1 €/kWh was assumed [26]. The total working costs can be calculated as the sum of the three energy costs and the effluent fines.

2.2. Principal component analysis

For statistical analysis with principal component analysis (PCA), the software program SPSS version 17 was used (www.ibm.com). PCA was used to select the most discriminating parameters and to investigate the overall variation of the data. PCA was used as pattern recognition method and aims at reducing a large number of variables to a smaller number of representative variables (principal components or PC's) [27]. Varimax normalised rotation of principal components was carried out in order to reduce the contribution of variables with minor significance and increase the interpretability of the components [27]. Initially 12 factors (influent flow rate, influent COD concentration, effluent COD concentration, dissolved oxygen set-point, effluent BOD concentration, effluent ammonium concentration, effluent nitrate concentration, effluent total nitrogen concentration, effluent suspended solids concentration, nitrate recycle flow rate, the sludge recycle flow rate and the waste flow rate) were used. The influent total nitrogen concentration was not considered as in this study it is related to the influent COD concentration. This relation would make the correlation matrix a non-positive definite matrix and would make further analysis such as the Bartlett test impossible.

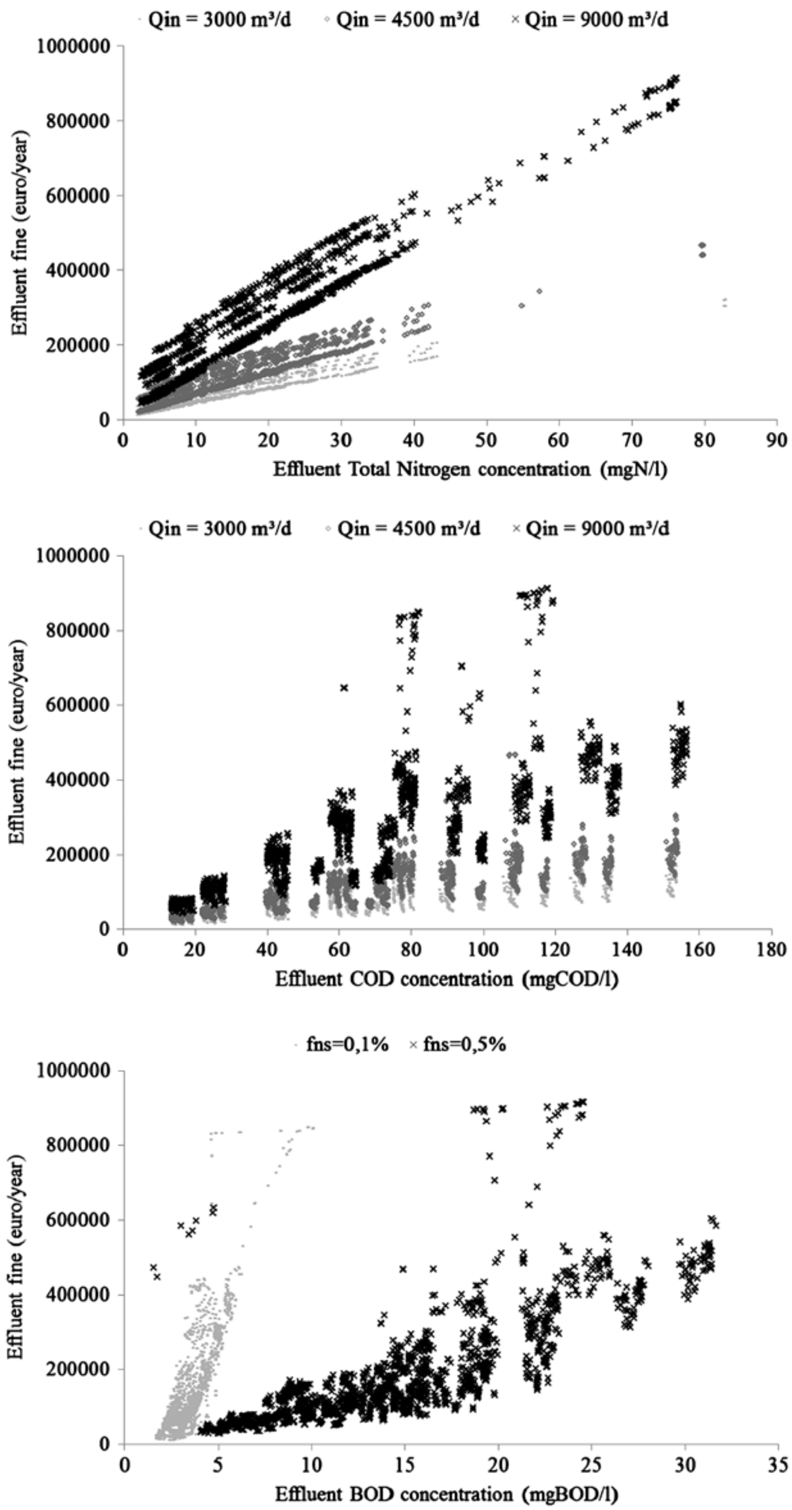

Fig. 2. Effluent fines (expressed as euro/year) as a function of the effluent concentration (expressed as mg/l). Top: total nitrogen concentration, middle: COD concentration and bottom: BOD concentration.

A first PCA analysis revealed that the correlation of the dissolved oxygen set-point with the other factors is too low (<0.4). As such, the dissolved oxygen set-point was not included in further statistical analysis and only 11 factors are considered further. The rule of thumb that the ratio "Cases to Factors" should be at least 5/1 is met with over 4,000 cases and 11 factors. The Kaiser–Meyer–Olkim criterion for sampling adequacy (KMO) and the Bartlett test were used to verify that correlations between items were sufficiently large for PCA. This KMO value should be above 0.5 [28].

The resulting PCA score plots are given as supplementary material and the main findings will be discussed in the results section.

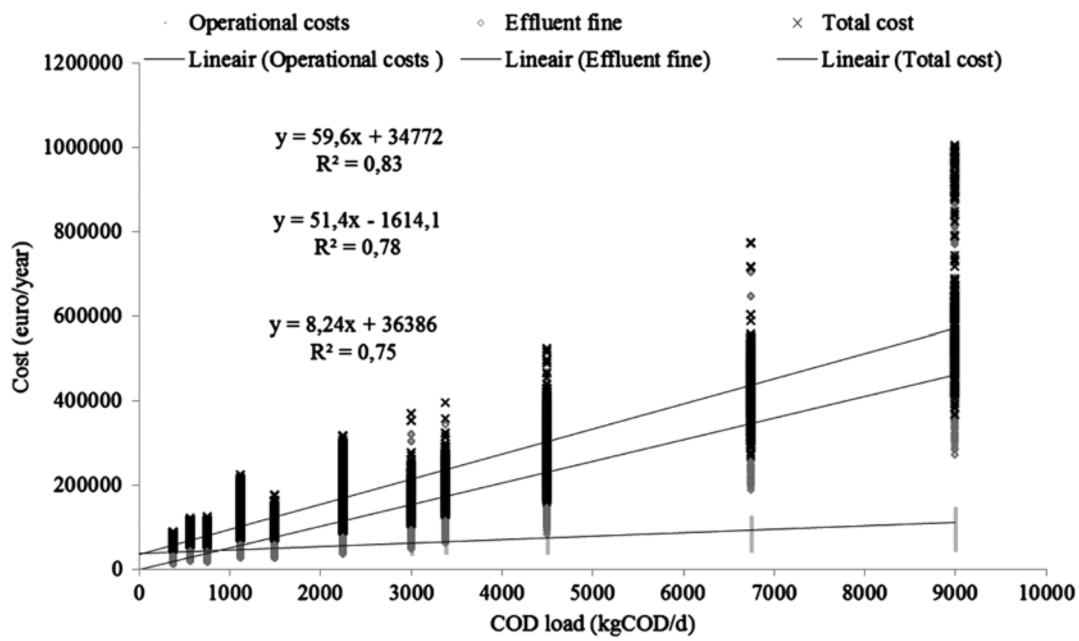

Fig. 3. The effluent fines, the operational cost and the total cost as function of the COD influent load.

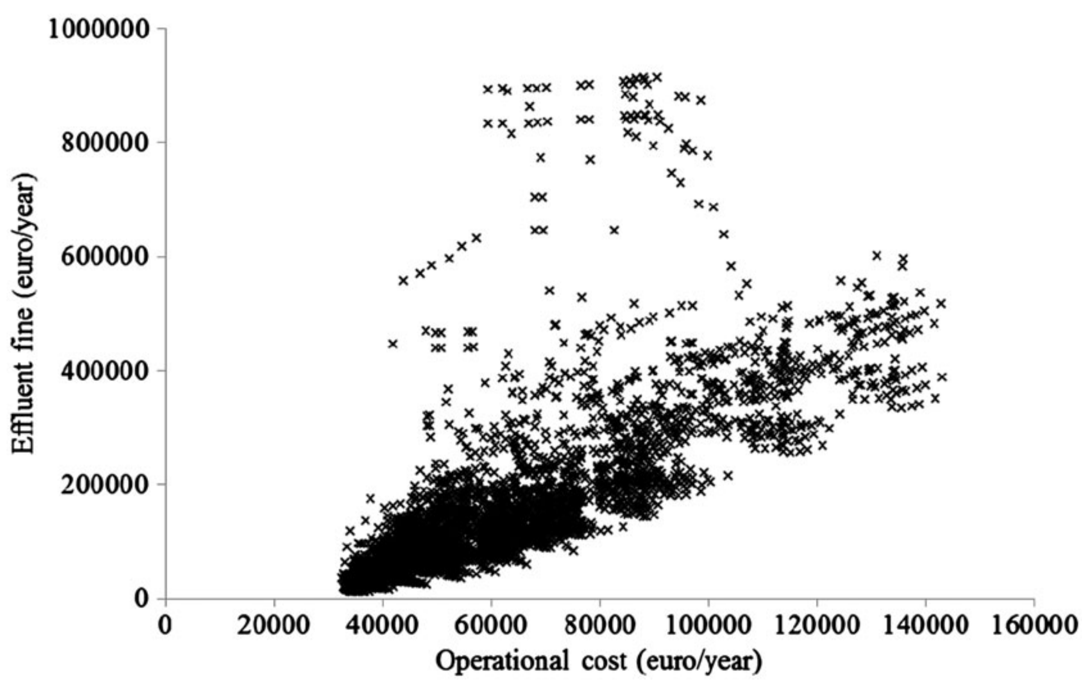

Fig. 4. Comparison between operational costs and effluent fines.

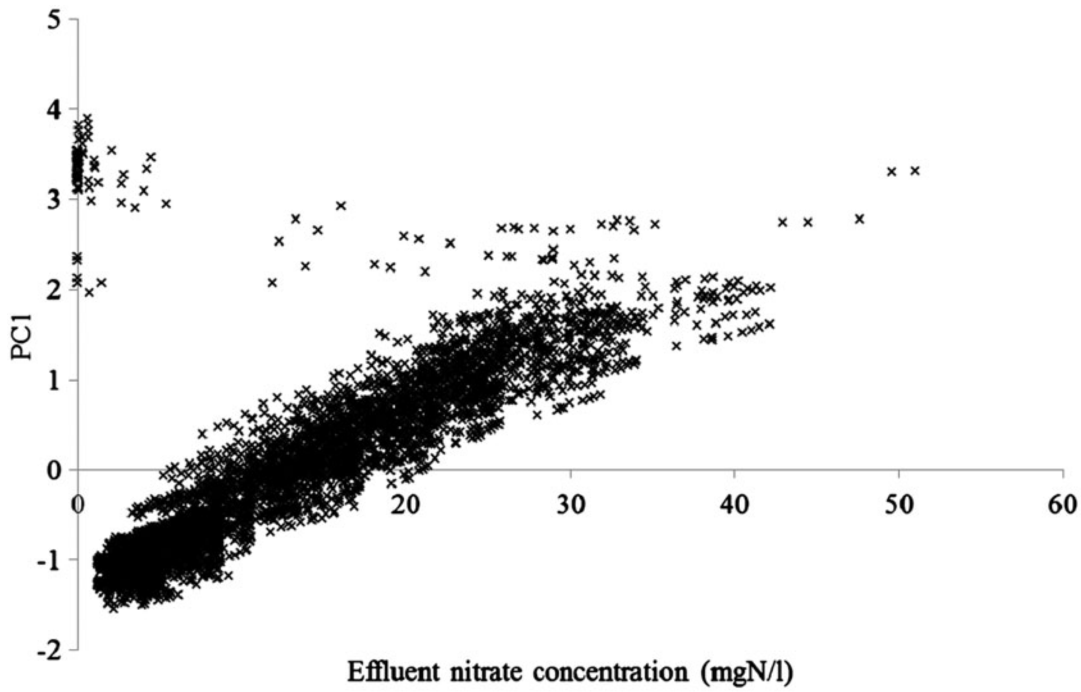

Fig. 5. The relation between effluent nitrate concentration and PC1.

3. Results

3.1. Scenario analysis results

3.1.1. Overall performance

In Table 2, the simulation results are compared to the discharge limits set by the Flemish government. In general, it can be seen that the WWTP design is rather robust for removing COD as only 10% of all simulation results result in a violation of the COD discharge limit (125 mg COD/l) and only 3% of all simulation results result in a violation of the BOD discharge limit (25 mg COD/l). Especially high COD influent

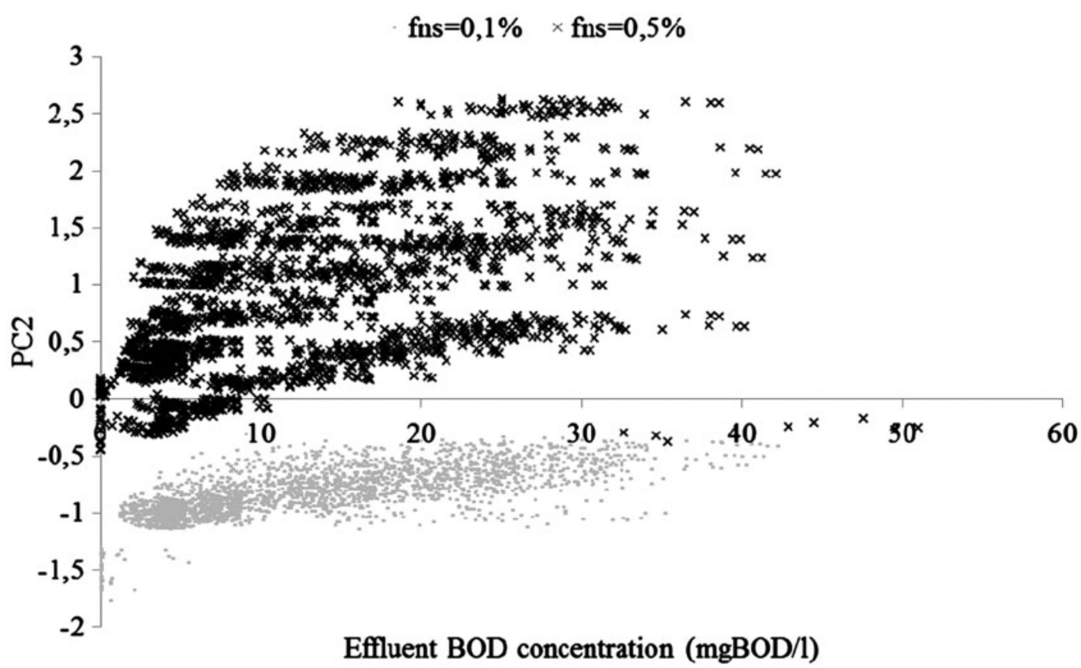

Fig. 6. The relation between effluent BOD concentration and PC2.

concentrations (>500 mg COD/l) led to a high (>85%) removal.

For total nitrogen and suspended solids removal, a different result is obtained as 42 and 35%, respectively, of all simulation results violate the discharge limit of 15 mg N/l and 35 mg/l, respectively. For suspended solids removal, this violation is mainly attributed to the scenarios related to a high value of the non-settleable fraction of the biomass (0.5%, see below). For total nitrogen removal, a combination of factors could lead to this violation. For example, a low dissolved oxygen set-point (2 mgO_2/l) combined with a low HRT (0.5 d) could lead to an increased total nitrogen concentration.

Concerning the energy use, it can be stated that the average energy consumption calculated over all simulations is 0.33 kWh per m^3 of water treated. This value was calculated based on the PE, the aeration energy and the ME. Further, this value is very similar to the average energy consumption of municipal WWTP installations in Flanders (Belgium): 0.3 kWh/m^3 [25].

3.1.2. Effluent fines

The effluent fines as a function of effluent concentration are depicted in Fig. 2. Logically, the effluent fines increase with increasing effluent concentration. As can be seen in Fig. 2, an important influencing factor is the influent flow rate, especially when the effluent fines are expressed in terms of effluent nitrogen concentration (Fig. 2, top and middle). However, the main influencing factor for effluent fines is the operation of the secondary settler, expressed in terms of the non-settleable fraction of the biomass (Fig. 2, bottom). If this fraction is high, then the COD, BOD and suspended solids effluent concentrations will also be high and this will result in a high effluent fine.

Table 3
The resulting rotated patterns of factors after varimax rotation.

Variable	Factor		
	1	2	3
Influent flow rate	0.12	0.05	*0.88*
Influent COD	*0.89*	0.27	−0.11
Effluent COD	0.41	*0.89*	−0.06
Effluent BOD	0.22	*0.91*	0.19
Effluent ammonium	0.47	−0.09	0.15
Effluent nitrate	0.76	0.25	−0.07
Effluent total nitrogen	*0.93*	0.12	0.06
Effluent Suspended solids	−0.18	*0.95*	0.003
Waste flow rate	*0.78*	−0.03	0.46
Nitrate recycle flow rate	0.01	0.04	*0.77*
Sludge recycle flow rate	0.06	0.01	*0.73*

3.1.3. Operational costs

In Fig. 3, the effluent fines, the operational cost and the total cost is depicted as function of the COD influent load. In can be seen that all costs will increase because of the effluent concentration, the pumping costs and the aeration costs will also increase. It should be noted that the slope of the effluent increase is five times higher than the slope of the operational costs increase this indicates that an increased load will affect the fines more than the operational costs.

In Fig. 4, the operational costs are compared to the effluent fines. Is can be seen that these two values are linearly related except for some points which was due to the absence of sufficient nitrogen removal caused by a low HRT and the effluent fines increase.

3.1.4. Principal components analysis (PCA)

The KMO value for the sampling adequacy of the PCA analysis was equal to 0.5. This indicates that correlations between items were sufficiently large to apply PCA [28]. This was confirmed by the Barlett's test of sphericity ($p < 0.05$). In Table 3, the resulting rotated pattern of principal components (after varimax rotation) is presented. It was decided to use the first three principal components which can explain 75% of the total variance of the simulate data. The first PC explained 37% of the variance, while the second and third PC explained 20 and 17% of the total variance, respectively.

The first principal component explains 37% of the total variance and contains most of the information on nitrogen removal as it is related to the effluent concentration of ammonium, nitrate and total nitrogen and the influent COD concentration. This is confirmed by the highlighted components in Table 3. The influent COD concentration is related to the amount of nitrate that can be denitrified. The relation between PC1 and nitrogen removal is illustrated in Fig. 5, where PC1 is plotted against the effluent nitrate concentration. A linear trend is observed.

The second principal component (PC2) explains 20% of the total variance and contains most of the information on the effluent COD, BOD and suspended solids concentration. As such, this principal

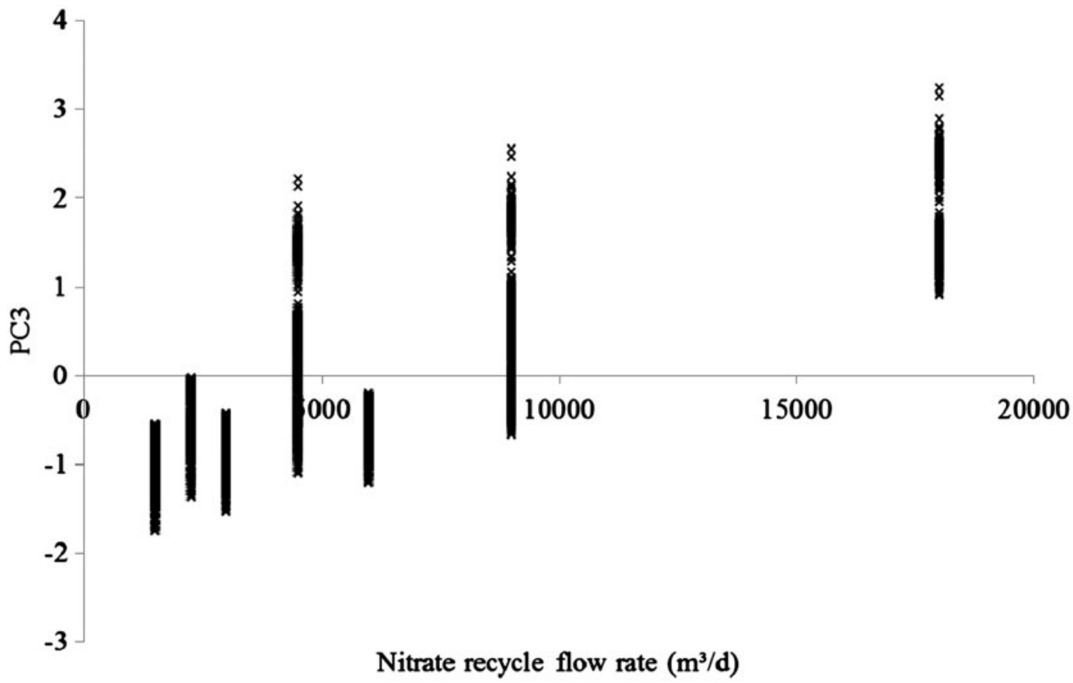

Fig. 7. The relation between the nitrate recycle flow rate and PC3.

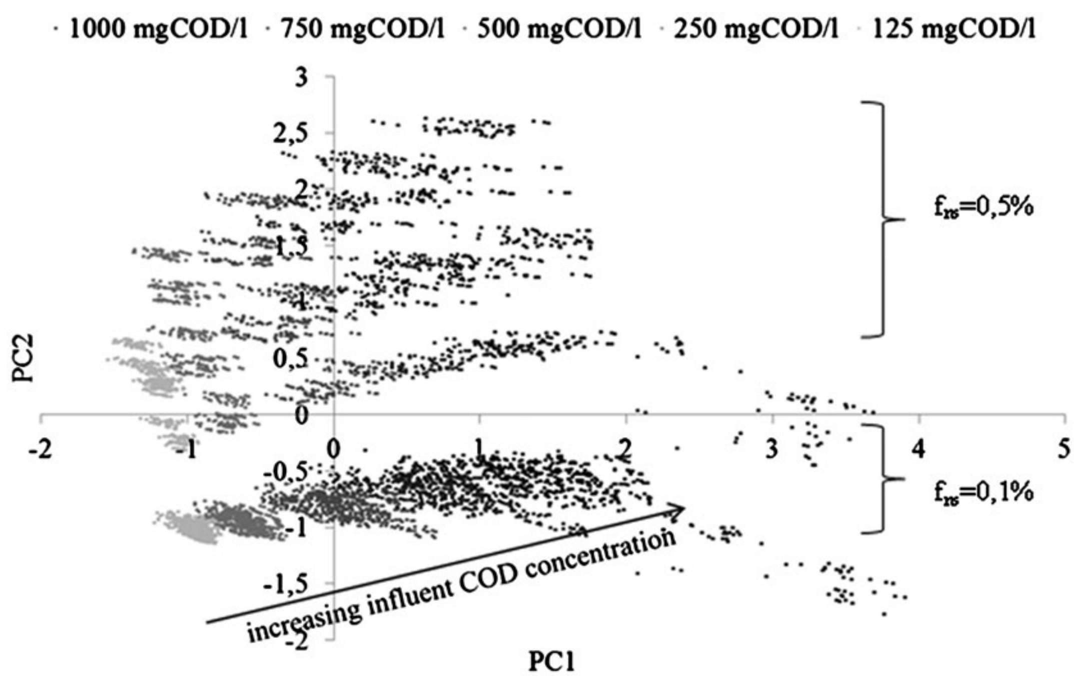

Fig. 8. Score plots of the PCA analysis, relating PC1 and PC2 to the influent COD concentration and the non-settleable fraction of the biomass (f_{ns}).

component can be considered as a measure of the secondary settler performance as these values will greatly be influenced by this performance. The relation between PC2 and settler performance is illustrated in Fig. 6, where PC2 is plotted against the effluent BOD concentration. An increase of the effluent concentration is noticed as function of the non-settleable fraction of the biomass (f_{ns}).

The third principal component (PC3) explains 17% of the total variance and mostly contains information on the different flow rates. This is illustrated in Fig. 7 in which the relation between PC3 and the nitrate recycle flow rate is depicted.

The relation between the two first principal components (PC1 and PC2), the influent COD concentration and the settler performance is depicted in Fig. 8. In this figure the increase in COD influent concentration is depicted in a grey scale (a darker colour indicates a higher influent concentration). An increasing PC1 coincides with an increasing influent COD concentration, while an increasing f_{ns} value coincides with an increasing PC2.

During PCA analysis the influence of dissolved oxygen set-point and the hydraulic regime, expressed by the number of tanks in series was investigated, but little or no effect was noticed (data not shown).

4. Conclusion

In this study, WWTP simulation results are interpreted in terms of system performance. The main influencing factors were found to be the influent flow rate and load, and the settler performance in terms of the non-settleable fraction of the biomass. This was further exemplified by a PCA analysis where three principal components were used. The first principal component explained 37% of the total variance and contains most of the information on nitrogen removal. The PC2 explains 20% of the total variance and can be considered as a measure of the secondary settler performance. The PC3 explains 17% of the total variance, and mostly contains information on the different flow rates in the WWTP (influent flow rate, nitrate recycle flow rate, sludge recycle flow rate and waste flow rate).

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