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Multi-criteria evaluation of control strategies in WWTP removing organic carbon, nitrogen and phosphorus

Xavier Flores-Alsina, Lluís Corominas and Peter A. Vanrolleghem
modelEAU, Département génie civil et génie des eaux. Université Laval. Pavillon Adrien-Pouliot, 1065, avenue de la Médecine. G1V0A6. Québec, QC, Canada.
e-mail: Peter.Vanrolleghem@gci.ulaval.ca

Abstract: The objective of this paper is to show the usefulness of multivariate statistical techniques to structure and visualize the information contained in multi-criteria matrixes obtained from the evaluation of control strategies in wastewater treatment plants (WWTP). The performance of sixteen different control strategies is evaluated by measuring their degree of satisfaction for twenty-four environmental, technical, economical and legal objectives using the "Neptune Simulation Benchmark" (an A_2O WWTP removing organic matter, nitrogen and phosphorus). Cluster analysis (CA), principal component /factor analysis (PCA/FA) and discriminant analysis (DA) are applied to the simulation output of the tested control strategies. The results of the case study show that multivariate analysis is a useful tool to straightforwardly differentiate WWTP control strategies with multiple criteria. Specifically, CA identified similar patterns in the alternatives with and without external chemical addition and/or TSS controller. Also, PCA/FA allowed discovering the main correlations between the evaluation criteria and the control strategies influencing those criteria most. Finally, thanks to DA it can be seen that from the original list of evaluation criteria, only a small sub-set of four, *i.e*. sludge production, aeration energy and time in violation of effluent limits for COD and P, cause the main differences in the overall process performance. Future evaluation of control strategy performance can therefore be restricted to an evaluation of only these four criteria.

Keywords: automatic control, benchmarking, cluster analysis, discriminant analysis, factorial analysis, multivariate analysis, nutrient removal

1. INTRODUCTION

Nutrient removal in Wastewater Treatment Plants (WWTPs) can be improved and optimised by implementing control strategies. Different control actions are possible (control of aeration, recirculation pumping, carbon addition, etc.) that allow improving/optimizing different aspects of the process (**Devisscher *et al*., 2002, Ingildsen and Olsson, 2002; Olsson *et al*., 2005; Thomsen and Önnerth, 2009**). The evaluation and comparison of different control alternatives is complex due to the fact that several factors have to be taken into account simultaneously, e.g. economic, environmental, technical, and legal aspects. The result is a complex evaluation matrix consisting of a large number of criteria that is difficult to interpret, thus making it difficult to draw meaningful conclusions.

Multivariate statistical techniques have been widely used as unbiased methods in analysis of complex data for extracting significant information (see for example **Johnson and Wichern (1992) and Hair *et al.* (1998)**). These techniques can be used to unravel the natural association between treatment alternatives, operating variables and evaluation criteria, thereby highlighting information not available at first glance. This paper aims to show how multivariate statistical techniques can mine the intensive multi-criteria evaluation matrixes and provide aggregate indicators that enhance the understanding of the whole evaluation procedure.

2. METHODS

2.1. Plant layout, model implemented control strategies and evaluation criteria

The *Neptune Simulation Benchmark* (NSB) was the activated sludge plant under study. The NSB design was conducted following the Metcalf & Eddy guidelines (**Metcalf & Eddy, 2003**). The plant layout is comprised of seven reactors in series (tanks ANAER1 & 2 are anaerobic with a total volume of 2000 m^3, tanks ANOX1 & 2 are anoxic with a total volume of 3000 m^3 and tanks AER1, AER2 & AER3 are aerobic with a total volume of 9000 m^3). These are linked with an internal recycle between the 3rd aerobic (AER3) and the 1st anoxic (ANOX1) tank. The secondary settler has a surface area of 1500 m^2 and a total volume of 6000 m^3. Further details about the NSB design and default (open loop) operational setting can be found in Deliverable 1.2 of the EU Neptune project (**www.eu-neptune.org).**

Simulations were performed using the WEST modelling environment (**MOSTforWATER NV, Kortrijk, Belgium**). The EAWAG Activated Sludge Model No 3 Bio-P was chosen as (bio) chemical model (**Rieger *et al*., 2001**). This model has 19 state variables and describes (bio) chemical phosphorus removal with simultaneous nitrification and denitrification in activated sludge systems by means of a large set of non-linear differential equations. The model was extended to include chemical precipitation of phosphorus as in ASM2d (**Henze *et al*., 2000**). The double exponential velocity function of **Takacs *et al*. (1991),** based on the solids flux concept was selected as a fair representation of the settling process, using a 10 layer discretisation. The kinetic parameters are adjusted according to the influent temperature using the Arrhenius equation. The default parameters for the activated sludge and the settling model can be found in **Rieger *et al*. (2001)** and **Copp (2002)** and the parameters for phosphorus precipitation kinetics were taken from **Gernaey *et al*. (2002**). It is important to highlight that the settling characteristics are assumed to be constant along the case study although the authors are aware that the floc characteristics may change in systems with chemical precipitation. Plant performance evaluation was based on a one year simulation with influent data generated according to the principles outlined in **Gernaey *et al*. (2006)** and adapted to the ASM3 Bio-P model.

Sixteen control strategies were implemented and compared to a default open loop base case (A_1). The control strategies [A = (A_2,...,A_{17})], summarized in **Table 1**, were applied to the activated sludge section of the WWTP. The simulation results (open loop case + 16 control strategies) were the starting point for the work presented in this paper. All simulations (609 days) were preceded by steady state simulations (200 days). Only the data generated during the last 364 days of simulation were used for plant performance evaluation.

Table 1 Control strategies evaluated in this case study (SP: set-point; * 3500 gTSS·m^{-3} in winter and 4000 gTSS·m^{-3} in summer (T>15ºC), Q_{intr}: internal recycle flow; Q_{carb}: Carbon addition flow; Q_w: wastage flow; Q_m: metal flow)

Charact.	**O_2**	**NH_4^+**	**NO_3^- (Q_{intr})**	**NO_3^- (Q_{carb})**	**TSS**	**Surmacz**	**PO_4^{-5}**
Reference	Olsson et al, 2002	Olsson et al., 2002	Olsson et al., 2002	Olsson et al, 2002	Olsson et al., 2002	Vanrolle ghem and Gillot 2002	Gernaey et al., 2002
Measured variable(s)	S_O AER1,2,3	S_{NH} AER3	S_{NO} ANOX2	S_{NO} ANOX2	TSS AER3	OUR AER1	S_{PO4} AER3
Controlled Variable(s)	S_O AER1,2,3	S_O SP AER1,2,3	S_{NO} ANOX2	S_{NO} ANOX2	TSS AER3	S_o SP AER1&2	S_{PO4} AER3
Set-point/ critical value	2 $gO_2\,m^{-3}$	1 gN·m^{-3}	1 gN·m^{-3}	1 g N·m^{-3}	3500 & 4000* g TSS·m^{-3}	650 gO_2·m^{-3}·d^{-1}	1 g P·m^{-3}
Manipulated variable	K_La	S_O SP	Q_{intr}	Q_{carb}	Q_w	S_O SP	Q_m
Control algorithm	PI	Cascaded PI	PI	PI	Cascaded PI	ON/OFF cascaded PI	PI
Control strategies	A_2-A_{17}	A_4, A_5, A_7, A_8, A_{10}, A_{11}	A_3, A_4, A_5, A_{12}, A_{13}	A_6, A_7, A_8, A_{14}, A_{15}	A_5, A_8, A_{11}, A_{13}, A_{15}, A_{17}	A_{12}-A_{17}	A_9, A_{10}, A_{11}, A_{16}, A_{17}

A set of evaluation criteria $X = X_1,....,X_{24}$ (see **Table 2**) was used to compare the different control strategies implemented in the NSB. The criteria include the effluent quality index (EQI) (taken from **Copp, 2002** and adapted to include effluent phosphorus with a weight of 10), the risk of suffering microbiology-related TSS separation problems (**Comas *et al.*, 2008**) and the original operational cost index (OCI), suggested by **Vanrolleghem and Gillot (2002)** adapted to include metal addition cost. The other criteria such as the time the plant is in violation for certain effluent limits (T_{viol}) can be found in **Copp (2002)**.

2.2. Multivariate statistical techniques

The work conducted here follows the methods applied in **Flores *et al.* (2007):**

Cluster analysis (CA) is an unsupervised pattern recognition technique that uncovers intrinsic structure or underlying behaviour in data without making a priori assumptions. Classification of the objects or a system into categories or clusters is based on the nearness or similarity of data points (e.g. **Hair *et al.*, 1998).** In this contribution hierarchical clustering is performed on the data set – after scaling the variables between 0 and 1 – by means of Ward's method, using the Euclidian distance as a measure of similarity.

Principal component Analysis (PCA) extracts the eigenvalues and eigenvectors from the covariance matrix of the autoscaled variables. The set of principal components (PCs) are the uncorrelated (orthogonal) variables obtained by multiplying the original correlated variables with the eigenvectors. Factor analysis (FA) further reduces the contribution of less significant variables obtained from PCA and results in the new groups of variables known as varifactors (VF) extracted through rotating the axis defined by PCA (**Hair et al. 1998**).

Discriminant Analysis (DA) is used to determine the variables (criteria) which allow discrimination between two or more naturally occurring groups (**Johnson and Wichern, 2002**). It operates on raw data and the technique constructs several discriminant functions identifying the most relevant criteria.

3. RESULTS

3.1. Cluster analysis

Figure 1 presents the dendogram with all implemented control strategies. Depending on the rescaled distance different levels of clustering are obtained. In the upper level, control strategies were grouped into three main statistically significant clusters (cluster 3.1, 3.2 and 3.3). The first cluster corresponds to strategies without chemicals addition (strategies A_1, A_2, A_3, A_4, A_5, A_{12} and A_{13}), the second groups strategies with metal addition (A_9, A_{10}, A_{11}, A_{16} and A_{17}) and the third corresponds to strategies with external carbon source addition (A_6, A_7, A_8, A_{14} and A_{15}). When the clusters are further classified, five groups of control strategies can be discerned (cluster 5.1, 5.2, 5.3, 5.4 and 5.5). Both clusters 3.2 and 3.3 are subdivided in clusters with (cluster 5.2 and 5.4) and without TSS control (cluster 5.3 and 5.5). Overall, the most important message after clustering is that there are five different types of control strategies, where the presence and the absence of external chemicals and /or a TSS controller are key elements creating the differences between the groups.

3.2. Principal component/factor analysis

PCA/FA was applied to the autoscaled simulation output to compare the evaluation criteria of the implemented control strategies and to identify the most influential factors. PCA of the entire data set resulted in four PCs with eigenvalues higher than 1. A varimax rotation of the PCs to the four corresponding VFs explained about 93 % of the total variance. The values of the PCs were further cleaned up with this technique and in the VFs the contribution of the original criteria could be identified more clearly.

The loadings (coefficients) of the evaluation criteria on the four first rotated PCs are presented in **Table 2**. The factor loadings were classified as "strong" (**bold**), "moderate" (*italics*) and "weak" corresponding to absolute loadings being >0.70, 0.70-0.50 and < 0.25.

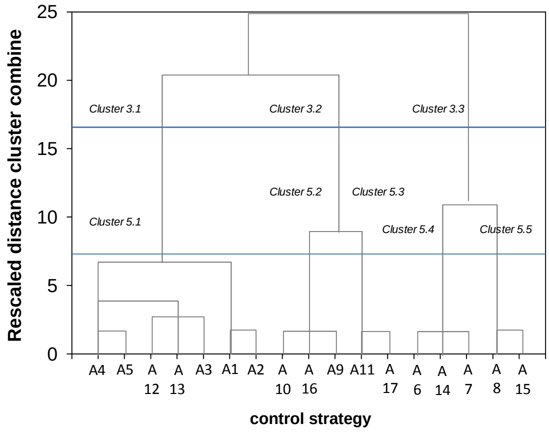

Figure 1. Dendogram showing clustering of the implemented control strategies in the Neptune

VF1, which explained 42.18 % of the total variance, had strong (in bold) positive loadings for X_5, X_6, X_7, X_9, X_{10}, X_{13}, X_{17}, X_{19}, X_{20} and strong negative loadings for X_2, X_{16}, X_{23}. This VF thus described the effect of the external carbon source addition. In fact, a periodic addition of an external carbon source (X_{13}) implies the subsequent increase of the sludge production (X_9) and aeration energy (X_{10}). In addition, there is a decrease of the effluent total nitrogen (X_2, X_{16}) as a direct consequence of the lower effluent nitrate concentrations). Nevertheless, negative impacts of the external carbon source addition are a decrease of the overall organic matter pollution removal efficiency (X_5, X_6, X_7, X_{17}, X_{19}, X_{20}), and a higher oxygen demand in the aerobic zone, i.e. higher aeration energy (X_{10}). Thus, operating conditions occurred that potentially could lead to low DO bulking (X_{23}). VF2 which explained 24.9 % of the total variation was positively correlated with X_3, X_4, X_8, X_{21} and negatively with X_{12}. This VF highlighted that with the addition of a metal salt (X_{12}) it is possible to achieve very low concentrations of phosphorus in the effluent (X_3, X_4, X_{21}) improving the overall wastewater treatment removal efficiency (X_8). Criteria X_1, X_{17}, X_{24} presented strong loadings in VF3 (19.7% of the total variance) indicating low nitrification efficiency. Finally, VF4, explaining 5.6 % of the total variance, had strong positive loading with mixing energy. The criteria X_{22} (bulking due to influent C and N disequilibrium) was not included in the analysis because it exhibited a constant value (i.e. variance zero).

Table 2. Loading of the evaluation criteria on the four first rotated PCs for the complete data set

		VF1	VF2	VF3	VF4
Total Kjeldahl Nitrogen (TKN)	X_1	0.03	-0.18	**0.91**	0.15
Total Nitrogen (TN)	X_2	**-0.81**	-0.02	-0.30	-0.33
Total Phosphate (SPO4)	X_3	-0.02	**0.99**	-0.12	0.04
Total Phosphorus (TP)	X_4	-0.03	**0.99**	-0.12	0.04
Chemical Oxygen Demand (COD)	X_5	**0.96**	0.24	0.00	0.06
Biochemical Oxygen Demand (BOD_5)	X_6	**0.93**	0.14	0.26	0.21
Total Suspended Solids (TSS)	X_7	**0.98**	-0.10	0.04	0.07
Effluent Quality Index (EQI)	X_8	-0.06	**0.99**	-0.08	0.01
Sludge Production (P_{sludge})	X_9	**0.70**	-0.24	*-0.61*	0.24
Aeration Energy (AE)	X_{10}	**0.71**	0.19	*-0.61*	-0.07
Pumping Energy (PE)	X_{11}	0.24	*-0.58*	0.55	0.18
Metal Salt (MS)	X_{12}	-0.30	**-0.93**	-0.09	-0.16
External Carbon Source (CS)	X_{13}	**0.75**	0.09	*0.61*	0.14
Mixing Energy (ME)	X_{14}	-0.16	-0.22	0.02	**-0.88**
Operational cost index (OCI)	X_{15}	*0.55*	*-0.66*	*0.64*	0.01
Nviolation (Limit = 18 g m^{-3})	X_{16}	**-0.86**	0.12	-0.09	0.13
COD violation (Limit = 100 g m^{-3})	X_{17}	**0.98**	0.00	-0.02	0.07
S_{NH} violation (Limit = 4 g m^{-3})	X_{18}	-0.16	-0.12	**0.95**	-0.11
TSS violation (Limit = 30 g m^{-3})	X_{19}	**0.98**	0.00	0.00	0.07
BOD_5 violation (Limit = 20 g m^{-3})	X_{20}	**0.98**	0.01	0.04	0.08
P violation (Limit = 2 g m^{-3})	X_{21}	0.19	**0.97**	0.02	0.13
DO deficiency bulking	X_{23}	**-0.77**	-0.10	-0.41	0.34
Low F/M bulking	X_{24}	-0.26	-0.04	**-0.84**	0.14

It is important to highlight the role that some moderate factor loadings (0.7 – 0.5) had in the created factorial model. For example X_9 and X_{10} had a moderate role in VF3. The correlation between (X_9) and (X_1, X_{18}) was mainly due to the improvement of the nitrification process when the airflow increases. Also, the increased sludge production (X_{10}) consequently decreased the F/M ratio and finally increased the risk of bulking due to low F/M. Another example was the influence of the operating cost index (X_{15}), which was relatively high in VF1, VF2 and VF3. Thus, the addition of either an external carbon source (VF1) or a metal salt (VF2) and higher aeration energy (VF3) increased costs.

Once the principal components were identified and labelled, the scores obtained by the implemented control strategies, can be calculated as a linear combination of the original criteria values. The representation of the scores is depicted in **Figure 2.** As expected, the results of PCA/FA were in good agreement with these of the CA. Control strategies with external carbon source (cluster 3.3) present high scores in VF1 (**Figure 2**, left) and are characterized by high operating costs and low effluent nitrate concentrations in the effluent. Cluster 3.2 presented high scores in VF2 (**Figure 2**, left) associated to the addition of a metal salt and low effluent phosphorus concentrations. This fact is attributed to the low soluble organic matter coming with the influent that makes a complete biological nitrogen removal really difficult without the addition of chemicals. Thus, in order to achieve low concentrations of nitrate and phosphates in the effluent it is necessary to add either external carbon source or metal salt. Strategies A_4, A_5 (with ammonia controller and without chemical addition) presented the highest nitrification efficiencies and therefore presented the lowest scores in VF3 (**Figure 2** right). Low scores in VF4 (**Figure 2**, right) were obtained for those strategies with an OUR controller (A_{12}, A_{13}, A_{14}, A_{15}, A_{16}, A_{17}) mainly due to the higher mixing energy consumption that is due to the activation/deactivation of the aeration system in the aerobic zone.

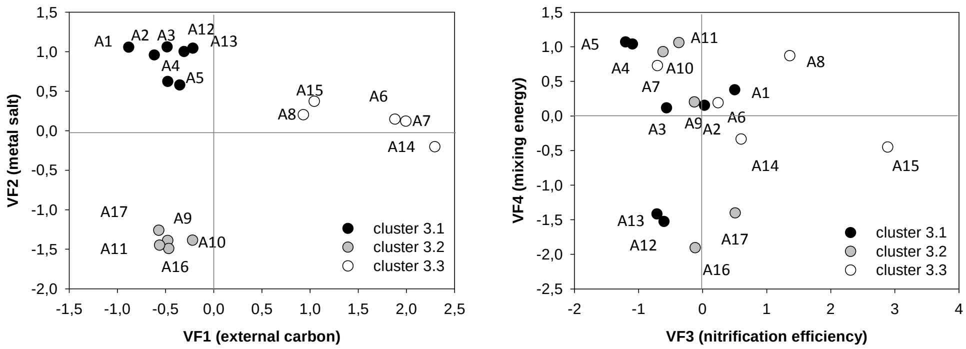

Figure 2. Principal component scores for the implemented control strategies for the principal component 1 and 2 (left) and for principal component 3 and 4 (right)

From the above we learn that PCA/FA helps us understanding the most important impacts of control strategies and their main interdependences. Thus, rather than evaluating the different control strategies in 24 dimensions, this approach drastically reduces the analysis to 4 VFs. These VFs explain the impact of the external carbon source (VF1), the addition of metal salt (VF2), the nitrification efficiency (VF3) and the mixing energy (VF4).

3.3. Discriminant Analysis

Finally, discriminant analysis (DA) was performed aiming at dividing the original data set into the three groups identified by CA, i.e. control strategies with and without chemical additions. The control strategy was the grouping variable, while all evaluation criteria were considered as independent variables. DA was performed using all evaluation criteria except X_{22} (again because of its null variance) and it rendered classification matrixes (CM) assigning 100 % of the cases correctly. The stepwise DA showed that criteria X_9, X_{10}, X_{17} and X_{21} were the discriminant variables. The correct grouping pattern of DA coincided with the clusters obtained in CA. Both CA and DA predict important differences in operational costs and plant performance due to the impact of the addition of chemicals. The discriminant functions are listed in **Table 3.**

Table 3. Classification functions for discriminant analysis of the implemented WWTP control strategies

	Description	D1	D2
X_9	Sludge production (P_{sludge})	1.32	1.37
X_{10}	Aeration energy (AE)	1.29	0.93
X_{17}	CODviolation	1.41	0.40
X_{21}	Pviolation	1.83	-0.08

Figure 3 represents the scores of each control strategy to the two determined discriminant functions (D). Thus, D1, with the highest discriminant ability separated cluster 3.2 from clusters 3.1 and 3.3. This is mainly due to the effect of the metal salt addition on the overall plant performance. The addition of the external carbon source explains the separation of cluster 3.1 and 3.3 as also shown in **Figure 3**. Thus, the message that can be extracted from this part is that sludge production (X_9), aeration energy (X_{10}), COD (X_{17}) and P (X_{21}) violation are the only four criteria that need to be looked at when comparing strategies, as these criteria had the highest discriminating power.

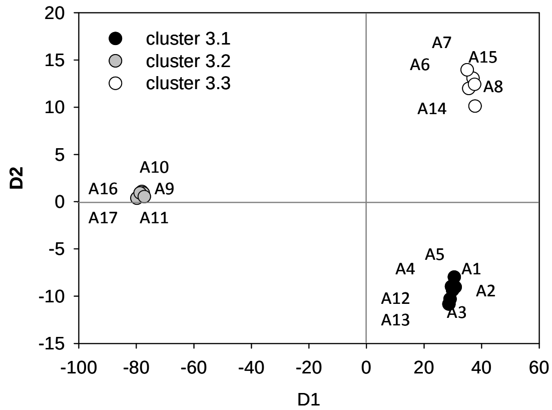

Figure 3. Classification functions for the discriminant analysis of the implemented control strategies

4. DISCUSSION

Overall, this analysis showed a straightforward way of characterizing alternatives. By looking at the clusters in some more detail, one can identify commonalities that allow generalization. For example, in case an environmentally friendly alternative is looked for, one would go for one of the control strategies within cluster 3.2 and 3.3, i.e. more expensive to operate but with lower eutrophication potential due to a reduced effluent N and P. On the other hand, if there are some budgetary limitations, the alternatives with the better chance of being successful are included in cluster 3.1. In the same way, it is possible to know in advance that switching from a metal salt controller (cluster 3.2) to an external carbon addition controller (cluster 3.3) will suppose a drastic increase in P violations. If this change is made from cluster 5.2 and 5.3 (external carbon) to 5.1 (no chemical addition) these differences lead to a substantial reduction of sludge production and aeration energy. This method thus provides process engineers, plant operators and decision makers more knowledge than current evaluation methods, highlighting pros and cons of each decision and enhancing the understanding of the whole evaluation process.

Some of the conclusions that arise concerning the control behaviour have to be taken with care and it may be dangerous to draw universal conclusions. For example, in some cases, it was found that the implementation of some controllers did not come up with either substantial cost reduction or effluent quality improvement to make the investment worthwhile, e.g. the OUR and ammonium controllers. The controllers presented in this paper were selected and combined in an arbitrary way and were not optimized, i.e. the values of the set-points were taken from literature. Hence, the simulations reflect the complex interactions amongst them. For this reason, they do not necessarily reflect their sole and true behaviour. Rather, the analysis methods presented here are intended as valuable research tools to coordinate the discussion and plan future research activities in order to assess the performance of some control strategies that improve nutrient removal.

Further research is envisaged by the authors to extend the analysis with additional simulations modifying the set-points of the proposed controllers in order to evaluate the implication of, for example, higher or lower oxygen, TSS, ammonia or nitrate concentrations in the bioreactors.

Another interesting point that can be extracted relates to the conceptualization of fault tolerant control strategies. For example, in the event that the NH_4^+ controller fails, the results of **Figure 2a** show that it can easily be deactivated temporally without substantial implications in terms of effluent TN and TP. Nevertheless, one should keep in mind that an increase of the effluent ammonia has to be expected in some cases (**Figure 2 left**). On the other hand, if either the external carbon source or the metal salt addition controllers fail, and no dosage occur for a while, a drastic deterioration in effluent quality will result.

Finally, the impact of the initial list of evaluation criteria should be mentioned. The results of the multivariate analysis show that redundant information is included within the set of criteria, and only few of the initial 24 criteria present a clear variation from one alternative to another. Nevertheless, the reader should be aware that it is impossible to know a priori which would be the main correlation between the evaluation criteria. Each PCA model is really case-specific and some changes may occur from one study to another, with different control strategies and evaluation criteria. For this reason, the authors advocate the use of the studied techniques to improve the interpretation to the information generated by assessing a multitude of criteria in view of an effective evaluation of control strategies. As a side effect, there is also a reduction in the cognitive load on the decision maker, yielding more knowledge than current evaluation methods provide and enhancing the understanding of the whole evaluation process.

5. CONCLUSIONS

The results of the multivariate analysis generated several conclusions.

i) Cluster analysis (CA) proved to be a useful tool offering reliable classification of groups of control strategies according to their behaviour for the Neptune benchmarking case study. CA performed this function well, rendering five groups of similar control strategies and identifying similar patterns in the control strategies with and without chemicals addition and/or TSS controller.

ii) Principal component analysis/factor analysis (PCA/FA) showed the main correlations between the evaluation criteria and the control strategies influencing those criteria. The four PCs identified were responsible for 93 % of the total variability (compared to 24 original criteria). As a result, various synergies were identified, e.g. carbon and metal addition correlate with higher nitrogen and phosphorus removal. Tradeoffs were also identified e.g. chemical addition against higher operating costs, carbon addition against worse organic matter pollution removal. In addition, with the results of the factorial scores, it was possible to identify the similarities between the implemented control strategies and the PCs extracted in the first part of the analysis. For example, alternatives with an ammonia controller were located in the VF3 that correlated with nitrification efficiency.

iii) Finally, discriminant analysis (DA) showed that only 4 criteria were needed to discriminate within the classes obtained by CA. Two discriminant functions were obtained, allowing 100% correct assignation and resulting in considerable data reduction. Analysis of the discriminant scores allowed finding the minimum set of criteria to differentiate the control strategies.

6. ACKNOWLEDGEMENTS

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