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# Predicting pollutant removal in constructed wetlands using artificial neural networks (ANNs)

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#### Abstract

Growth in urban population, urbanisation, and economic development has increased the demand for water, especially in water-scarce regions. Therefore, sustainable approaches to water management are needed to cope with the effects of the urbanisation on the water environment. This study aimed to design novel configurations of tidal-flow vertical subsurface flow constructed wetlands (VFCWs) for treating urban stormwater. A series of laboratory experiments were conducted with semi-synthetic influent stormwater to examine the effects of the design and operation variables on the performance of the VFCWs and to identify optimal design and operational strategies, as well as maintenance requirements. The results show that the VFCWs can significantly reduce pollutants in urban stormwater, and that pollutant removal was related to specific VFCW designs. Models based on the artificial neural network (ANN) method were built using inputs derived from data exploratory techniques, such as analysis of variance (ANOVA) and principal component analysis (PCA). It was found that PCA reduced the dimensionality of input variables obtained from different experimental design conditions. The results show a satisfactory generalisation for predicting nitrogen and phosphorus removal with fewer variable inputs, indicating that monitoring costs and time can be reduced.

*Keywords:* Constructed wetlands; Urban stormwater; Pollutant removal; Artificial neural networks (ANNs); Principal component analysis (PCA)

# 1. Introduction

According to the United Nations (2018), over 55% of the world's population lives in urban areas, a proportion that is expected to increase to about 68% by 2050. With increasing urbanisation, the demand for water increases, especially in water-scarce regions. Therefore, to increase water availability, interventions such as a reduction in water consumption, reclamation of water sources, and sustainable treatment of wastewater (recycling and reuse) has been proposed. Constructed wetlands (CWs) have been increasingly used in wastewater treatment, partly because the construction and maintenance costs of CWs are relatively low. Additionally, CWs can hold and treat variable volumes of wastewater, thus mitigating extreme weather conditions (floods and droughts) associated with climate change. Moreover, the process of pollutant removal in CWs occurs through a combination of biological, chemical, and physical processes (Wynn and Liehr, 2001; Lee et al., 2002; Langergraber et al., 2008), which enables CWs to treat various types of wastewater. However, understanding such multifaceted processes is complex and requires advanced analytical tools such as computational models (Langergraber, 2007). Previous modelling studies on the pollutant removal in CWs were mainly based on hydraulics and nutrient biogeochemistry (Kadlec, 2000; Wynn and Liehr, 2001; Langergraber and Simunek, 2005; Langergraber et al., 2008; Akratos et al., 2009). Likewise, the ecological behaviour in polluted water bodies was explored by integrating hydrodynamic models and neural networks to collate physical, chemical, and biological interactions that underpinned the different processes (Lin et al., 2008).

More recently, numerical models, such as AQUASIM, HYDRUS, and STELLA, have been used to describe contaminant adsorption phenomena in CWs treating municipal wastewater (Mburu et al., 2012, 2014). Those studies show that obtaining boundary conditions to represent wastewater treatment in CWs as well as to describe treatment processes can be challenging. Additionally, due to the different modelling and wetland design criteria, it is difficult to compare the performance of different CWs. Specifically, HYDRUS is unable to simulate CWs operated through a

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tidal-flow strategy due to the inflexibility of the model to varying boundary conditions in a single modelling scenario. For instance, while Lucas et al. (2015) demonstrated that HYDRUS could predict the biologically influenced removal processes of ammonia nitrogen ( $NH_4^+$ -N), it was unable to model the removal of orthophosphate ( $PO_4^{3-}$ -P) using the same technique.

However, methods such as the artificial neural network (ANN) model have emerged as powerful data mining tools. ANNs can identify complex patterns from various data formats, which has led to the increase of ANN implementations in multiple fields, including tumour and cancer detection in the healthcare sector, audio and image recognition in digital accessories such as smartphones, and machine language translation on internet search engines. ANNs perform best when dealing with nonlinear univariate and multivariate data. In hydro-environmental studies, ANNs have been used to predict the biochemical oxygen demand (BOD) and suspended solids (SS) concentrations in the effluent of a wastewater treatment plant (Hamed et al., 2004); BOD and chemical oxygen demand (COD) removal in horizontal subsurface flow constructed wetlands (HFCWs) (Akratos et al., 2008); stormwater quality (May and Sivakumar, 2009; May et al., 2009); and the removal of PO<sub>4</sub><sup>3-</sup>-P, total nitrogen (TN), and total phosphorus (TP) in HFCWs (Akratos et al., 2009). For the design of CWs, the mechanistic models can be limited by several factors, including the operational strategy deployed to the wetland treatment system and the difficulties in measuring the definitive boundary conditions. There is a need to develop simple yet effective methods for evaluating the overall performance of a pollution control strategy when designing CWs. Specifically, the black-box nature of wastewater treatment in CWs makes the ANN approach an appropriate modelling technique, but its performance depends on the selection of input variables and the network architecture accounting for the size, nature, and type of the input data. To make the ANN-based simulations more effective, the multiple variables in large datasets need to be grouped to identify the relationships among the variables using multivariate methods such as principal component analysis (PCA) (Herngren et al., 2006; Gunawardana et al., 2014), which describes the complete data matrix with a reduced number of principal components by transforming the original variables into a new orthogonal set of principal components for defining the relationships among the variables. The aim of this study was to develop an ANN model to optimise the novel configurations of vertical subsurface flow constructed wetlands (VFCWs) for treatment of stormwater and to predict nitrogen and phosphorus removal using influent-effluent data obtained from laboratory experiments.

# 2. Methods

In order to develop a model based on ANN, a series of laboratory experiments were carried out over a continuous period of two years (2014 – 2016) using eight pilot-scale VFCWs. VFCWs are wastewater treatment systems designed as pre-treatment units in horizontal flow beds (Seidel, 1965). VFCWs are common in Austria, Denmark, France, and the UK, and are deployed in treating stormwater. They are preferred to HFCWs because VFCWs have minimal land requirements. VFCWs usually contain macrophytes rooted in the bed media (gravel or loamy sand) compacted to a depth between 0.6 m and 1.0 m (Fig. 1). VFCWs are mostly intermittently dosed (Langergraber et al., 2008) and can be operated either as planted or unplanted, with some studies reporting that planted VFCWs had enhanced pollutant removal rates (Taylor et al., 2011). Plants are reported to provide favourable environments that facilitate the growth of microbial populations and the release of oxygen into the treatment system (Wang et al., 2012, Wu et al., 2015), thus enabling the biological removal of nitrogen and phosphorus (Zhu et al., 2012). Driven by gravity, wastewater in VFCWs flows down gradually through the media bed, thus enabling oxygen to transfer from the atmosphere into the media. Oxygen facilitates the nitrification of nitrogen products (Cooper et al., 1996), leading to better removal of organics, SS, and  $NH_4^+$ -N . However, VFCWs are not suitable for denitrification as  $NH_4^+$ -N is usually converted into nitrate nitrogen ( $NO_3^-$ -N).

# 2.1. Experimental setup

Eight pilot-scale VFCW units were set up on the roof of South Building at the School of Engineering of Cardiff University. Each VFCW unit used in the experiments was moulded from a structured-wall high-density polyethene (HDPE) pipe with a height of 1000 mm and a diameter of 400 mm. Each unit was sealed off at the bottom using an HDPE plastic fitted with a drainage tap at the centre (Fig. 1). Different biofilter media were used to configure the VFCW in various design units. All the units were planted with *Typha latifolia*.



(a) Physical model

(b) Size and typical layout

Fig. 1. Experimental setup of VFCW units

In this paper the results from six VFCW units out of eight are presented because the data collected from the other two VFCW units that were intermittently operated are not sufficient for the ANN modelling technique. Units 1, 4, 5, and 7 were filled with loamy sand, while units 2 and 8 contained fine gravel and blast furnace slag media, respectively (Table 1). Semi-synthetic stormwater was used to conduct the experiments partly because of the complex logistics of procuring large volumes of natural stormwater, and the absence of SS, colloidal matter, and artefacts in synthetic stormwater (Akratos and Tsihrintzis, 2007).

Table 1

Media configurations in VFCW units.

Unit	Primary media	Transition media	Drainage media
1, 4, 5, 7	Loamy sand	Sharp sand	Fine gravel
2	Fine gravel	Medium gravel	Coarse gravel
8	Blast furnace slag	Sharp sand	Fine gravel

Semi-synthetic stormwater was prepared by mixing natural sediment with tap water dechlorinated using sodium thiosulphate. Natural sediment was collected from a stormwater pond in Nant y Briwnant (Cardiff) and from gulley pots in the car park at the School of Engineering of Cardiff University. Sediments were wet-sieved through a 1 mm-diameter sieve, and hence the particle sizes were comparable to those in pre-treated stormwater (FAWB, 2009). Contaminant concentrations in the resulting slurry were analysed in the Characterisation Laboratories for Environmental Engineering Research (CLEER), at the School of Engineering of Cardiff University. In some cases laboratory-grade chemicals (K<sub>2</sub>HPO<sub>4</sub>, NH<sub>4</sub>Cl, Pb(NO<sub>3</sub>)<sub>2</sub>, ZnSO<sub>4</sub>·7H<sub>2</sub>O, CuCl<sub>2</sub>·2H<sub>2</sub>O, Cd solution (1000 mg/L), Cr(NO<sub>3</sub>)<sub>3</sub>, NiCl<sub>2</sub>·6H<sub>2</sub>O, and FeCl<sub>2</sub>·4H<sub>2</sub>O) were added to attain influent pollutant concentrations typical of UK urban areas.

## 2.2. Operation, sampling, and analysis

All six VFCW units were tidal-flow operated on three consecutive days of each experimental week. Tidal flow is a technique used to operate VFCWs, and it is characterised by the unidirectional movement of wastewater (Lavrova and Koumanova, 2013). The feeding of the semi-synthetic stormwater stops as the surface is fully submerged and flooded. The media bed holds the wastewater until a set time is reached, and then it starts to drain downward. Loads of semi-synthetic influent stormwater was slowly and gently dosed on the media surfaces of each VFCW units. The treatment cycle is completed when effluents are fully drained from the filtration bed, and air (oxygen) is drawn in and allowed to diffuse into voids in the biofilters (Bruch et al., 2014).

The VFCW units are usually designed based on the wetland-watershed area ratio (WWAR), where the surface area is determined as a percentage of the size of the watershed area. However, because the design of stormwater VFCWs varies with the amount of rainfall received and the treatment requirements in different catchments, there are no specific WWAR design codes. Nevertheless, standard guidelines and recommendations have typical WWARs of 1%–5%; while WWARs of 2%–3% are recommended in the UK (Ellis et al., 2003). Thus, any WWAR that minimises land

requirements without compromising performance can be used, especially where retrofitting of the system is planned.

In this study, units 1, 2, 4, and 8 were operated at a 2.5% WWAR, while units 5 and 7 had 5.0% and 1.5% WWARs, respectively. The VFCW units with WWARs of 2.5%, 5.0%, and 1.5% received stormwater loads in batches of 22.5 L, 11.3 L, and 37.6 L, respectively, and the stormwater was held in the VFCW units for 24 h. Before feeding the VFCW units, 300 mL of the influent stock was taken, and in-situ measurements of pH, temperature, and electrical conductivity (EC) were recorded with a multi-parameter HANNA Probe (Model HI 991301). After the 24-h retention period, effluent samples were collected using the outlet tap on each VFCW unit. Effluent in-situ readings were taken, and the effluent samples prepared for analysis and storage at 4°C in a fridge in the CLEER laboratory. Chemical water parameters such as the concentrations of TN,  $NH_4^+$ -N, nitrite nitrogen ( $NO_2^-$ -N),  $NO_3^-$ -N,  $PO_4^{3-}$ -P, TP, and total suspended solids (TSS) were analysed using a spectrophotometer (Hach Lange DR3900) based on pollutant specified standard methods (APHA, 2012). Similarly, the analysis of heavy metals such as Cu, Pb, Cd, Cr, Ni, and Fe was carried out in the CLEER laboratory using the inductively coupled plasma optical emission spectrometer (ICP-OES, Optima 210 DV, PerkinElmer).

# 2.3. Data

Data for the daily and weekly influent-effluent pollutant concentrations were converted into monthly averages to obtain representative treatment efficiency of each VFCW unit. The monthly data were considered good indicators because it took nearly three months for the VFCWs to attain treatment stability. Thus, the initial experimental data (0 to 150 d) were excluded from the analysis. All the experimental data were pre-processed and examined to establish trends, relationships, and data dependencies.

Exploratory data analysis revealed multiple nonlinear combinations among the variables (27 in total, including derived variables such as the percentage reduction), which followed exponential patterns. The complexity and nonlinearity exhibited by the dataset also suggested that ANNs are a suitable analytical tool. Significant differences were found in the means of the variables, and some variables exhibited non-normal distribution. The dataset comprising pH, EC, temperature, and the concentrations of TN,  $NH_4^+$ -N,  $NO_2^-$ -N,  $NO_3^-$ -N,  $PO_4^{3-}$ -P, and TP was re-scaled to achieve normal distribution and data components that could suitably explain the variance of the inputs. Due to the size and nonlinearity of the variables, PCA was used to extract the principal components (Herngren et al., 2006; Gunawardana et al., 2014), and the principal components were consequently used in the simulation to build ANNs to predict the performance of different designs.

# 2.4. Artificial neural networks

Wastewater treatment in CWs is often described as black-box and exhibits nonlinear characteristics. Consequently, the performance of CWs can be simulated using ANNs. ANNs are a form of artificial intelligence, which imitate the functioning of the biological nervous system. ANNs perform complex computations through training on inputs to produce outputs. Thus, ANNs can be used to model environmental systems, in which the key processes are challenging to quantify.

Although ANNs can be implemented through various network architectures, multi-layer perceptron (MLP) ANNs have been applied (Lin et al., 2008; Akratos et al., 2009; Abyaneh, 2014; Bagheri et al., 2015; Li et al., 2015; Lyu et al., 2018). MLPs consist of three distinct layers: input, hidden, and output layers (Fig. 2). The input and output layers can operate with any number of input variables such that neurons in both the input and hidden layers assess output responses concerning the weighted sum of inputs based on the activation function (Dawson et al., 2006). In this study, inputs were extracted using the PCA module in SPSS IBM 23 (George and Mallery, 2016), while the ANNs were implemented in winGamma (Jones et al., 2000). All the PCA-extracted variables for modelling TN and TP removal had no direct relationship with the outputs. The reliability of the ANN model was enhanced by eliminating derived inputs (percentage reductions) from the PCA. Similarly, the effect of inputs on the outputs (local sensitivity analysis) was evaluated using the model built from all the extracted principal components. Equally, to ensure a uniform modelling process, the experimental data were standardised, randomised, and partitioned into training (70%) and validation (30%), so that each data point could influence both the training and validation processes. Subsequently, underfitting or overfitting were minimised through application of the Gamma statistic and M-test, respectively (Jones et al., 2000). The algorithm

implemented in winGamma is a modified Broyden-Fletcher-Goldfarb-Shanno (BFGS) method, in which the BFGS adjusts network weights and thresholds to minimise training and prediction errors. Accordingly, the root mean square error (RMSE) was used to assess both the training (TRMSE) and validation (VRMSE) errors. Similarly, the coefficient of determination ( $R^2$ ) and the Nash-Sutcliffe efficiency (NSE) were used to evaluate the precision and efficiency of the ANN model, respectively.



Fig. 2. MLP networks with two hidden layers

# 3. Results and discussion

Table 2 shows the experimental data, including the mean values of each parameter and the standard deviation (SD), where *n* is the number of the samples, and *C* means the concentration. The results measured from six units, namely units 1, 4, 2, 8, 5, and 7, are presented. Units 1 and 4 represent the experimental control units operated at a 2.5% WWAR with loamy sand media. Similarly, units 2 and 8 were operated at a 2.5% WWAR, but with fine gravel and blast furnace slag media, respectively, while units 5 and 7 underwent experiments carried out at 5.0% and 1.5% WWARs, respectively, using the loamy sand. It can be noted that some parameters, mostly the heavy metals in the effluent, had concentrations below the detection limit (bdl) of the measuring instruments.

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Parameter	Influent	Unit 1	Unit 4	Unit 2	Unit 8	Unit 5	Unit 7	n
pН	$7.5\pm0.3$	$6.9\pm0.2$	$6.8\pm0.3$	$7.5\pm0.3$	$8.5\pm0.5$	$7.0 \pm 0.2$	$6.9\pm0.2$	183
Temperature (°C)	$16.4\pm4.0$	$16.4\pm3.0$	$15.2\pm4.0$	$15.5\pm3.0$	$15.0\pm4.0$	$15.3\pm4.0$	$15.2\pm4.0$	183
EC (mS/cm)	0.35±0.03	$0.62 \pm 0.04$	$0.61\pm0.06$	$0.37\pm0.04$	$0.47\pm0.08$	$0.57\pm0.06$	$0.57\pm0.05$	183
C(TSS) (mg/L)	167 ± 31	$15 \pm 11$	$7\pm3$	$8\pm3$	$9\pm4$	$15\pm9$	$11\pm9$	183
$C(PO_4^{3-}-P)(mg/L)$	$0.83 \pm 0.10$	$0.11{\pm}0.10$	$0.11\pm0.10$	$0.22\pm0.10$	$0.23\pm0.10$	$008\pm0.04$	$0.16\pm0.10$	183
<i>C</i> (TP) (mg/L)	$1.04\pm0.10$	$0.22\pm0.10$	$0.22\pm0.10$	$0.35\pm0.10$	$0.30\pm0.10$	$0.16\pm0.06$	$0.26\pm0.10$	183
$C($ NO $_2^-$ -N $)$ (mg/L)	$0.01\pm0.02$	bdl	bdl	bdl	bdl	bdl	bdl	183
C( NO <sub>3</sub> <sup>-</sup> -N $) (mg/L)$	$0.01\pm0.10$	$0.24\pm0.30$	$0.17\pm0.20$	$0.72\pm0.40$	$0.20\pm0.20$	$0.2\pm0.40$	$0.29\pm0.20$	195
$C(NH_4^+-N)(mg/L)$	$1.02\pm0.20$	$0.12\pm0.10$	$0.10\pm0.04$	$0.07\pm0.03$	$0.07\pm0.03$	$0.12\pm0.04$	$0.13\pm0.10$	195
<i>C</i> (TN) (mg/L)	$5.45 \pm 1.00$	$1.10\pm0.60$	$1.09\pm0.58$	$1.11\pm0.60$	$1.18\pm0.53$	$1.24 \pm 1.00$	$1.59\pm0.80$	183
<i>C</i> (Fe) (mg/L)	$3.35\pm0.90$	$0.11\pm0.10$	$0.04\pm0.10$	$0.09\pm0.10$	$0.043\pm0.04$	$0.108\pm0.10$	0.06 ±0.10	234
C(Zn) (mg/L)	$0.43\pm0.20$	$0.11\pm0.10$	$0.11\pm0.10$	$0.02\pm0.02$	$0.01\pm0.02$	$0.10\pm0.05$	$0.06\pm0.10$	234
<i>C</i> (Cu) (mg/L)	0.15	bdl	bdl	bdl	bdl	bdl	bdl	156
<i>C</i> (Pb) (mg/L)	0.6	0.005	0.001	0.11	0.0003	0.0007	bdl	156
<i>C</i> (Cr) (mg/L)	0.03	bdl	bdl	bdl	bdl	bdl	bdl	144
<i>C</i> (Cd) (mg/L)	0.004	bdl	bdl	bdl	bdl	bdl	bdl	159
<i>C</i> (Ni) (mg/L)	0.097	bdl	bdl	bdl	bdl	bdl	bdl	156

# 3.1. Design performance

Fig. 3 shows the percentage changes of pH, EC, Fe concentration, and Zn concentration measured in the effluent against the influent in different media over a period of 369 d from the 154th day of the experiments. The results from two settings of loamy sand media in units 1 and 4 (denoted as LS-1 and LS-4), fine gravel (FG), and blast furnace slag (BFS) media are included, where the influent values are also indicated for reference.



Fig. 3. Percentage changes of pH, EC, Fe concentration, and Zn concentration in effluent against influent in different media As shown in Fig. 3(a), the influent stormwater had pH values ranging from 7.0 to 8.0 with a high degree of consistency in the procedure used in preparing the semi-synthetic stormwater. The measured pH values for all media were highly consistent. The pH values in loamy sand (LS-1 and LS-4) were measured at around 90% of that of influent, while the pH in fine gravel was largely kept the same level as the influent. However, the pH value in blast furnace slag was higher than in the influent, which was due to the high pH level in the media. Nevertheless, it exhibited a decreasing trend. This clearly indicated that the effluent pH level depended on the influent pH, as well as the primary media type. Consequently, the pH values are found to be significantly lower in loamy sand and fine gravel as compared to blast furnace slag (p = 0.000, where p is the measure of statistical significance at a 5% confidence level, the probability of rejecting the null hypothesis) because the predominantly alkaline chemical composition of blast furnace slag changed significantly due to dilution and washout caused by repeated dosing and treatment events.

As shown in Fig. 3(b), the influent EC varied between 0.3 mS/cm and 0.4 mS/cm, with an average of 0.35 mS/cm. The mean effluent EC values from the experiments were measured as 0.37 mS/cm, 0.47 mS/cm, and 0.59 mS/cm in fine gravel, blast furnace slag, and loamy sand VFCW units, respectively, which were all higher than influent EC, with a significant increase of effluent EC by 150%–200% in loamy sand media and 120%–155% in blast furnace slag media from that in fine gravel media (p = 0.000), which was almost the same as the influent EC. The results indicated a significant difference in the efficiency with which the primary media filtered the suspended solids.

The concentrations of some pollutants in effluents exhibited values below the respective limits of detection, as evidenced by the heavy metals Cu, Pb, Cd, Cr, and Ni, which were almost completely removed. However, the removal rate of Fe was significant in all media, exceeding 90%, as shown in Fig. 3(c), with higher removal rates in loamy sand media. The removal rate of Zn, as shown in Fig. 3(d), was also significant, exceeding 55% in all the media types. There was a substantially high removal efficiency (up to 95%) for the period of around 318 d, particularly for the fine gravel and blast furnace slag media, and then a slight decrease to reach a steady reduction of 70% to 80%. Therefore, the removal rates of both Fe and Zn were high in general.

Fig. 4 shows the percentage changes of the concentrations of Fe, Zn, TP, and TN in units 1, 5, and 7, representing the WWARs of 2.5%, 5.0%, and 1.5%, respectively. It was found that the lower WWAR resulted in higher removal rates of Fe and Zn, as shown in Fig. 4(a) and (b) toward the end of the experiments, exhibiting a statistically significant difference (p = 0.000). The measurements also show that WWARs had little effect on the removal of Fe, but the effect of the WWAR on the removal of Zn was significant (p = 0.001). Although there is no monotonic increasing trend for the removal of Zn related to a higher WWAR, the cumulative mass load removal of Zn shows that the Zn removal rate was higher at a 1.5% WWAR (85.0%) and at a 2.5% WWAR (82.0%) in comparison with the 5.0% WWAR (71.0%). However, the effects of the WWAR on the removal of TN and TP, as shown in Fig. 4(c) and (d), were less evident, despite the significant reduction mostly being below 20%. Of the three cases, LS-5 was the most efficient media in the removal of TP and TN.



Fig. 4. Percentage changes of Fe, Zn, TP, and TN in loamy sand media with different WWARs

In the experiments, the influent temperature ranged between 6.8°C and 256°C and it was found that in general the effluent temperature was about 1°C lower than that of the influent without significant differences between the various designs. Influent TSS used in this study was highly variable between 79 mg/L and 290 mg/L (with an average of 167 mg/L), much lower than the 4 000 mg/L used in the VFCWs investigated by Torrens et al. (2009) and the 400 mg/L to 700 mg/L of Abdelhakeem et al. (2016). The effluent TSS in all VFCWs ranged from 7 mg/L to 15 mg/L, which was significantly lower than the influent TSS. Consequently, the cumulative mass removal rates of TSS almost reached 90% in all VFCWs, demonstrating adequate filtering capacity of loamy sand, fine gravel, and blast furnace slag primary biofilters. However, significant differences in TSS removal were found between different media, with the removal rates in the blast furnace slag media and fine gravel media higher than the average value in the loamy sand media (Table 3). The WWARs were also found to be a significant factor in TSS removal, with the highest removal rate at a 5.0% WWAR, compared to that at the 1.5% WWAR and the average value at the 2.5% WWAR, similar to the Fe and Zn removal.

Table 3Cumulative mass removal rate of pollutants in different VFCW units.

Unit	Removal rate (%)								
-	TSS	$PO_4^{3-}-P$	TP	$NH_4^+$ -N	TN	Fe	Zn		
1	91.4	87.2	80.2	88.6	81.0	96.9	76.4		

4	95.8	87.3	80.3	91.3	81.2	98.9 Jc	urnal Pre-proof
2	95.5	73.9	67.3	93.7	80.1	97.3	96.1
8	94.5	73.1	72.1	93.4	79.1	98.8	98.6
5	95.6	95.0	92.4	94.2	88.6	98.4	88.5
7	89.9	71.2	62.2	79.9	56.3	97.0	80.3

#### 3.2. Total nitrogen removal

The ANN-based models were built, using optimal inputs, to predict the removal of nitrogen and phosphorus nutrients. The selection of the optimal input parameters was achieved using PCA, local sensitivity analyses, and training and validation techniques. The details of the models are presented.

For TN removal, the models used different combinations of input parameters extracted from PCA, including influent SS, effluent Zn, effluent pH, influent  $NH_4^+$ -N, influent Fe, influent  $NO_3^-$ -N, and influent  $NO_2^-$ -N. The performance of the ANN models for the various simulated scenarios is listed in Table 4 for Unit 1 in terms of TRMSE, VRMSE,  $R^2$ , and NSE. The results clearly show the different effects of different combinations of inputs on the outputs as determined through local sensitivity analyses. Models 1 and 2 had comparable TRMSE and VRMSE values.

#### Table 4 ANN models for predicting TN removal in VFCW Unit 1.

Model	Network input variables	TRMSE	VRMSE	$R^2$	NSE
1	ISS, EZn, EpH, IAM, IFe, IN3, IN2	0.042	0.059	0.81	0.79
2	ISS, EZn, EpH, IAM, IFe, IN3	0.066	0.068	0.74	0.65
3	ISS, EZn, EpH, IAM, IFe, IN2	0.046	0.101	0.50	0.39
4	ISS, EZn, EpH, IAM, IN3	0.049	0.077	0.69	0.65
5	ISS, EpH, IAM, IN3	0.060	0.083	0.65	0.59
6	ISS, EZn, EpH, IN3	0.048	0.173	0.20	0.06
7	ISS, EZn, EpH, IAM	0.048	0.136	0.30	0.20

Note: ISS means influent SS, EZn means effluent Zn, EpH means effluent pH, IAM means influent  $NH_4^+$ -N, IFe means influent Fe, IN3 means influent  $NO_3^-$ -N, and IN2 means influent  $NO_2^-$ -N.

However, masking input influent  $NO_2^-N$  resulted in declines in  $R^2$  (8.6%) and NSE (17.7%) in the outputs of Model 2 (Table 4). Likewise, fewer inputs (models 3 through 7) did not improve the performance of the ANN model greatly. The variations of the outputs (TN removal) are mainly attributed to influent  $NO_3^-N$ , suggesting that influent  $NO_3^-N$  is key to TN removal in Unit 1. A comparison of the experimental and predicted TN removal rates in Unit 1 is shown in Fig. 5.



Fig. 5. Predictions of TN removal in Unit 1 with ANN model.

Similarly, ANN-based models were built to predict TN removal in units 2, 4, 5, 7, and 8 using the approach applied to Unit 1. For the models built for TN removal in units 4, 7, and 8, a similar number of predictors and low  $R^2$  and NSE values were obtained. TN removal predictions in Unit 8, as shown in Table 5, had low NSE, which could suggest inconsistencies

in the TN removal mechanism in blast furnace slag media. In fine gravel media (Unit 2), the TN removal rate was found to be consistently low (not shown here), which could be due to the limited TN removal mechanism, while in the loamy sand units, the relationship between TN removal and other inputs was variable even between the control units 1 and 4.

# Table 5

ANN models for predicting TN removal in VFCW Unit 8.

Model	Network input variables	TRMSE	VRMSE	$R^2$	NSE
1	IOP, ESS, ETR, EN3, EFe, ITP, EZn, IN2	0.042	0.174	0.25	0.21
2	IOP, ESS, ETR, EN3, EFe, ITP, EZn	0.042	0.086	0.53	0.40
3	IOP, ESS, ETR, EN3, EFe, ITP	0.039	0.099	0.54	0.51
4	IOP, ESS, ETR, EFe, ITP	0.050	0.074	0.67	0.63
5	IOP, ESS, ETR, EFe	0.053	0.068	0.71	0.65
6	IOP, ESS, ETR	0.068	0.072	0.68	0.44

Note: IOP means influent  $PO_4^{3-}$ -P, ESS means effluent SS, ETR means effluent temperature, EN3 means effluent  $NO_3^{-}$ -N, EFe means effluent Fe, and ITP means influent TP.

In summary, predictions of TN removal in all VFCWs brought  $R^2$  higher than 0.65, revealing a strong correlation with the experimental data. However, the NSE was variable. Specifically, the model for predicting TN removal in Unit 5, despite containing more input variables, had a higher error margin than the prediction errors produced by other models, while the model for TN removal in Unit 2 had fewer inputs and produced fewer errors with modest  $R^2$  and NSE values, as listed in Table 6. Comparatively, in blast furnace slag media, the ANN model had the lowest accuracy.

#### Table 6

Performance of ANNs in predicting TN removal in units 1, 2, 4, 5, 7, and 8 in comparison with experimental results.

Unit	Network input variables	Experimental removal rate (%)	Predicted removal rate (%)	Difference (%)	$R^2$	NSE
1	ISS, EpH, IAM, IN3	78.14	76.97	-1.17	0.65	0.59
2	IpH, ETR, IAM	61.87	61.70	-0.17	0.70	0.60
4	EOP, IOP, EEC	80.06	78.49	-1.57	0.73	0.54
5	ESS, EEC, EN3, ISS, IN2, IFe	73.07	71.41	-1.66	0.71	0.69
7	EOP, ISS, IZn	73.03	72.04	-0.99	0.73	0.61
8	IOP, ESS, ETR	78.95	77.42	-1.53	0.68	0.44

Note: IpH means influent pH, EOP means effluent PO<sub>4</sub><sup>3-</sup>-P , EEC means effluent EC, and IZn means influent Zn.

Generally, the data obtained from all VFCW units yielded ANN models with fewer input variables than the inputs identified through PCA, suggesting that TN removal can be monitored indirectly. Moreover, the ANN models predicted the TN removal rate with both TRMSE and VRMSE of less than 4% in all designs as shown in Table 5. Therefore, the generalisations derived by ANNs are satisfactory with regard to removal in the tidal-flow VFCWs. Nonetheless, better models could be developed using nonlinear data reduction techniques than PCA.

# 3.3. Predicting total phosphorus removal

Predictions of TP removal were derived from the inputs listed in Table 7 for Unit 1. Nitrogen species constituted the most predictors, as well as influent SS and influent Fe, reinforcing the theory that TP and SS removal tend to occur through similar mechanism of filtration and sedimentation. Nonetheless, the ANN models created from different inputs gave variable output ranges. Except for model 6, in which effluent TN was masked, the rest of the ANN models had low values of TRMSE and VRMSE. Thus, effluent TN significantly influenced the precision and reliability of the models. Unfortunately, no remarkable improvements in ANN performances were observed when the number of input variables was reduced.

Table	7		т		1	D		
ANN models for predicting TP removal in Unit 1. Journal P								
Model	Network input variables	TRMSE	VRMSE	$R^2$	NSE			
1	ESS, ETN, ISS, IAM, EN2, IFe, IN3	0.038	0.043	0.76	0.75			
2	ESS, ETN, ISS, IAM, EN2	0.038	0.047	0.74	0.73			
3	ESS, ETN, ISS, IAM, EN2, IN3	0.047	0.042	0.75	0.69			
4	ESS, ETN, ISS, IAM, EN2	0.033	0.062	0.66	0.65			
5	ESS, ETN, ISS, IAM, IFe, IN3	0.033	0.073	0.58	0.56			
6	ESS, ISS, IAM, EN2, IFe, IN3	0.029	0.110	0.20	0.13			
7	ETN, ISS, IAM, EN2, IFe, IN3	0.039	0.086	0.57	0.52			
8	ESS, ETN, ISS, EN2, IFe, IN3	0.044	0.048	0.69	0.64			

Note: ETN means effluent TN, and EN2 means effluent NO2-N.

The same procedure was applied to other VFCW units to examine the performance of the models in predicting TP removal with several input variable combinations. All the models exhibited robust generalisations with both TRMSE and VRMSE. TP removal obtained by the ANN models for units 5 and 7 showed better performance. Additionally, apart from Unit 4, TP removal representative models of all the other VFCW units were developed from fewer inputs relative to their respective standard models. Thus, regarding the media types, loamy sand VFCW units 1, 4, 5, and 7 produced good results, as shown in Table 8, while both blast furnace slag and fine gravel VFCW units produced weak models.

#### Table 8

Predicting TP removal in units 1, 4, 5, and 7.

Uni	t Network input variables	TRMSE	VRMSE	$R^2$	NSE
1	ESS, ETN, ISS, IAM, EN2	0.038	0.047	0.74	0.73
4	IpH, EZn, EEC, ESS, IN3, EFe	0.032	0.052	0.73	0.62
5	ESS, EN3, ETN, ISS, EpH	0.024	0.024	0.83	0.80
7	ETN, ITR, ISS, EAM, IAM	0.050	0.048	0.83	0.81

Note: EAM means effluent NH4-N , and ITR means influent temperature.

Table 8 shows the comparisons of the predicted TP removal rate from the best model with the experimental data in units 1, 4, 5, and 7 for the loamy sand with different WWARs where units 1 and 4 are the control units. It is clear that the TP removal rates predicted by the model agrees with the experimental data in general. Among the loamy sand VFCW units, the differences in performance could be attributed to variations in WWARs. At a 2.5% WWAR (units 1 and 4) the TP removal models performed well, but the TP removal rates attained by the 5.0% (Unit 5) and 1.5% (Unit 7) WWARs were better judged by the values of  $R^2$  and NSE. Thus, the cumulative TP mass removal rate was highest at a 5.0% WWAR (92%), followed by a 2.5% WWAR (80%), and lowest at a 1.5% WWAR (62%), as shown in Table 3. Similarly, the differences in the removal of TP for different VFCW units were found to be significant (p = 0.000). Furthermore, the Tukey post hoc test revealed that TP removal rate was significantly lower at a 1.5% WWAR in comparison with the 2.5% and 5.0% WWARs. Thus, the ANN models for predicting TP removal reflect these variations, and the results suggest that a lower TP removal rate occurs through specific removal mechanism. This explained the consistency observed, with the higher TP removal rate indicating the involvement of various factors and removal processes.

# 3.4. Discussion of ANN models for predicting TN and TP removal

The extracted principal components revealed that although all six VFCW units treated the same influent stormwater, each VFCW unit produced data specific to its design. Consequently, the developed ANN models had varying generalisations. Additionally, the principal components extracted to predict TN removal and TP removal differed for different VFCW units. This suggests that the relationships between the input and output variables are dependent on factors such as air temperature, and design and operation variables.

The initial objective to develop ANN models was to predict the removal rates of time-consuming and costlier-to-monitor pollutants (heavy metals, TP, and TN) from the relatively cheaper-to-monitor parameters (pH, temperature, and conductivity). However, the exploratory data analyses revealed significant differences between the means of the input variables. Moreover, most of the variables exhibited non-normal distribution.

Additionally, temperature, pH, and EC had a weak relation with the target outputs (TN removal and TP removal), which may be an indication that physical water quality is insufficient to characterise the dynamics of TN and TP removal in the VFCWs. Thus, PCA was found to be necessary to reduce the dimensions of the data and to identify the most significant inputs for building ANN models subsequently. VFCW units configured using loamy sand media yielded reliable model performances for TN and TP removal. However, fine gravel and blast furnace slag media exhibited extremely nonlinear patterns, which likely influenced the quality of the ANNs.

The best performing models of the VFCW units investigated in this study produced ANNs with considerably low training and validation error margins for TN removal, resulting in satisfactory generalisations. Furthermore, predictions of TN removal had all  $R^2$  values greater than 0.65, indicating a strong correlation between the predicted and experimental data. Except for units 1 and 5, the ANN models for predicting the TN removal rate in units 2, 4, 7, and 8 required few input variables, and the predictions were least reliable in Unit 8, perhaps because of the various TN removal mechanisms. Therefore, the long-term monitoring of the performance of TN removal in VFCWs can be achieved with ANNs. Similarly, it is possible to build more reliable ANN models for predicting TN removal by identifying significant input variables using nonlinear data reduction methods instead of PCA. ANN models for predicting TP removal contained more input variables than the TN removal models, suggesting that TP removal in VFCWs is more stochastic than TN removal.

However, no reliable model was developed for the fine gravel and blast furnace slag VFCWs, and only loamy sand VFCWs produced consistent or predictable TP removal. Nevertheless, ANN model predictions revealed meaningful variations in TP reduction in the loamy sand VFCWs. The differences in TP removal could be attributed to changes in WWARs. Thus, the models for TP removal with the 2.5% WWAR (units 1 and 4) performed better when compared with the models for Unit 5 (5.0% WWAR) and Unit 7 (1.5% WWAR). This shows that TP removal was consistent at higher WWARs as the influents were held longest due to the larger surface area available to small inflow volumes, while for lower WWARs (1.5% WWAR), less water could be withheld for a shorter treatment time, resulting in a lower reduction of TP. Although different media may yield different TN and TP removal performances, the results showed that the fine gravel and blast furnace slag media exhibited high nonlinearity, which in turn may influence the quality of the ANN models generated.

The results of the ANN models built from data of the control units 1 and 4 (loamy sand VFCWs) showed no significant difference in TN and TP removal rates, which indicates that the long-term pollutant removal in VFCWs can be strongly influenced by the primary media type and WWARs.

# 4. Conclusions

A series of laboratory experiments were continuously carried out over a two-year period. The water quality of effluents from six pilot-scale VFCW units, which were fed with semi-synthetic influent stormwater, was analysed. ANN models for predicting TN and TP removal in the VFCW units were developed from the most significant influent-effluent input variables identified through innovative exploratory data analyses.

The results show that primary media distinctly affected the changes in pH, EC, and removal of TP and TN in the investigated designs. However, all the media adequately reduced the pollutants in the stormwater. Specifically, blast furnace slag media attained higher removal rates of more pollutants than loamy sand and fine gravel media. However, loamy sand was most effective in removing TP, especially at a 5.0% WWAR, while fine gravel had the same efficiency in removing TN. The differences in the performance of loamy sand VFCWs were found to relate to the WWAR, but further study may be required to establish this relation for fine gravel and blast furnace slag media.

Similarly, the results of the ANN models for predicting TP and TN removal revealed satisfactory generalisations, showing agreement between the predicted and experimental data. Thus, ANNs are a useful tool for modelling pollutant removal in VFCWs. Furthermore, implementing nonlinear data reduction techniques could improve the reliability of the ANN models and reduce simulation time, as well as reduce input-output data requirements. Moreover, future research

should implement other ANN optimisation strategies like the radial basis function and machine learning.

However, scaling up the results from this study can be challenging, as the physical processes that convert rainfall to runoff are variable and challenging to replicate. Assumptions were also made for the hydraulic loading volumes derived from average annual rainfall rather than the rainfall intensity, and the retention time used in this study (24 h) excluded the situations of longer (> 24 h) rainfall events. Therefore, field studies must be conducted to complement the findings of this study before scaling up for engineering applications. Nonetheless, this study highlighted the effect of long and fixed retention time on pollutant removal in tidal-flow VFCWs.

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