

MODELLING THE PERFORMANCE OF WATER TREATMENT PLANTS USING ARTIFICIAL NEURAL NETWORKS – A LITERATURE REVIEW

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ABSTRACT

Since the 1990s the Artificial Neural Network (ANN) modelling approach has gained popularity for prediction and forecasting due to its ability to capture complex nonlinear relationships. The application of ANNs in the field of water treatment has been somewhat limited to date but the technique could prove to be a powerful tool in creating accurate models for predicting the performance of water treatment plants. In this paper, literature regarding modelling water treatment plant performance or a similar field of study has been assessed with the goal to establish the current state of creating an overall predictive water treatment plant model and identify knowledge gaps. A secondary goal is to establish a best practice for the modelling of water treatment plant performance. Only papers which helped in establishing the current state have been considered and this narrowed the number of assessed papers to 35. Modelling methods other than ANNs have also been reviewed and in conclusion insight has been gained in producing an overall water treatment plant model with model input selection and the generalisation ability being important aspects of the model and model development.

KEYWORDS

Modelling, Artificial Neural Network, Water Treatment Plant, Review

1 INTRODUCTION

With rising populations, increased industrial and agricultural water usage, and climate changes come challenges to supply water of adequate quality and in sufficient quantities. Due to this growing pressure, the water treatment industry now has a greater emphasis on the optimisation of water treatment plants to improve capacity, quality, operational costs and capital expenditure (Bozkurt et al., 2014). Operation has become increasingly more complex over the past few decades as new technology has been developed and regulations have been tightened.

The technologies utilised in water treatment can be energy intensive and costly, and a methodology which can predict plant performance and other key performance indicators is often lacking (Akinmolayan et al., 2015). Such a methodology could be beneficial to gain insight on different design and operating alternatives, identifying potential bottlenecks, and improve the operation of the water treatment plant by having a better understanding of the individual treatment processes. Modelling the water treatment plant performance may provide these benefits.

The modelling of water treatment plants is an area of interest for water suppliers for its prediction and forecasting abilities. It is a cost-effective method to identify potential future capacity issues and could prove a powerful tool for long-term capital planning.

The challenge in modelling water treatment plant performance is the complex dynamic nonlinear behaviour of water treatment systems. Traditional modelling methods like mathematical models, least squares regression and partial differential equations may be able to show general trends but often struggle predicting the outcome of specific events, making these models of less value for capital planning.

A modelling method which has gained significant popularity since the 1990s is the artificial neural networks (ANN) approach. ANNs are capable of finding highly complex nonlinear relationships, the produced relationship, however, will be of low transparency, making it hard to grasp the actual relationship produced. This, in combination with the results not physically being measured, is a major barrier for the water treatment industry to adopt implementation of models within water treatment plant control.

Although ANNs have gained popularity, only 8 of the 83 papers published between 2000 and 2014 about ANNs in the water treatment industry focused on water treatment performance (Wu et al., 2014).

In this paper an overview will be given on traditional modelling methods and their applicability and flaws to accurately predict and forecast water treatment performance. The application of ANNs on water treatment modelling or equal fields will be discussed, including the applicability to a complete predictive water treatment plant model.

2 OVERVIEW OF PAPERS REVIEWED

The year of publication of the articles considered has been plotted in Figure 1. There is a fairly even distribution of articles published in each year. As the overall goal was to gather information on creating a complete predictive water treatment plant model, articles which did not share valuable insight or recommendations were excluded. A large number of papers regarding modelling water treatment performance were statements of work done and did not discuss recommendations for future work. These kind of articles were not reviewed in this paper.

As the number of articles regarding modelling water treatment performance was limited, a few articles in areas similar with cross-over knowledge were included in this review. Figure 2 shows an overview of the distribution of articles by industry or area.

Figure 1: Distribution of papers reviewed by year of publication.

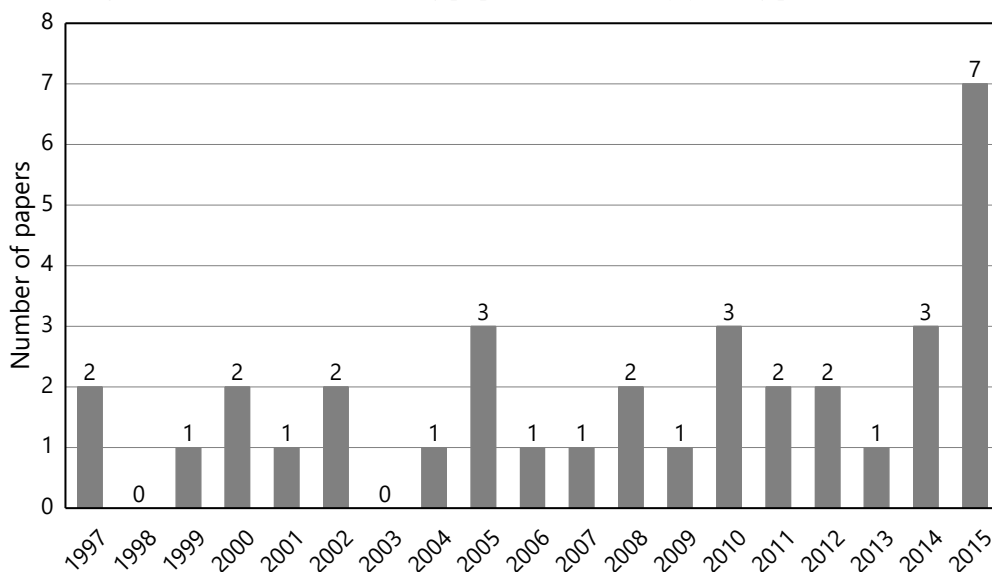
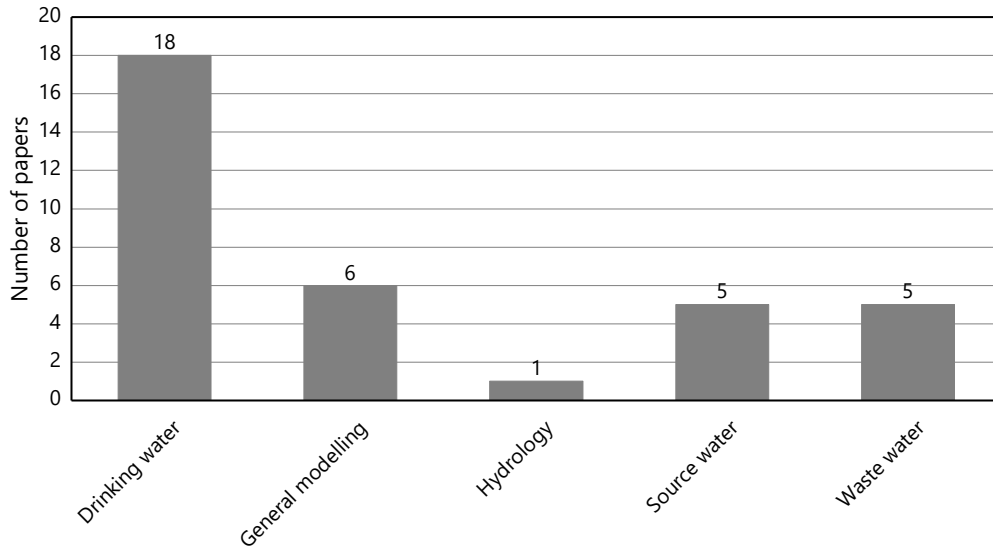


Figure 2: Distribution of papers reviewed by industry or area.



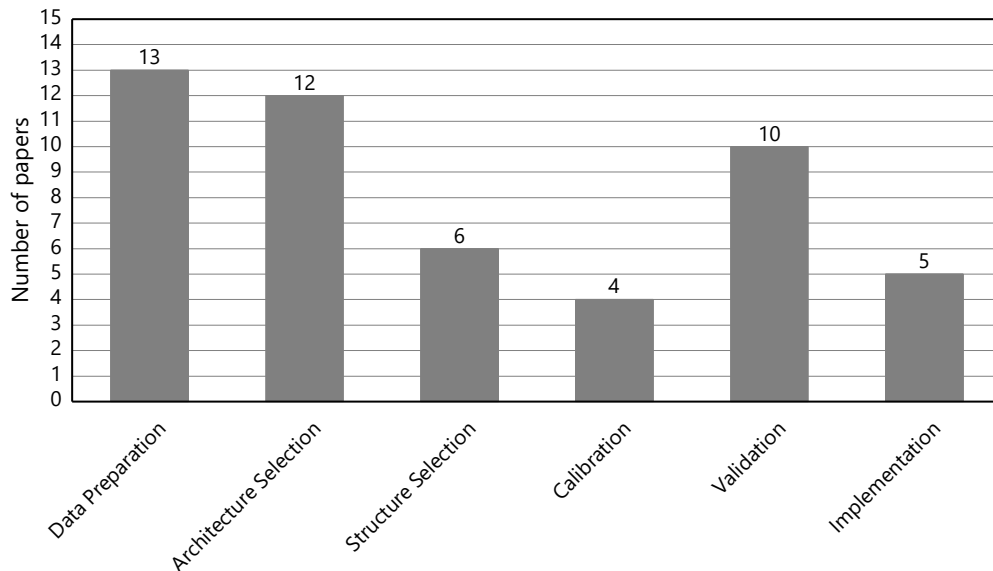
3 REVIEW OF PAPERS

One of the goals of this article was to have an overview of past modelling efforts on water treatment plants. Modelling is usually done in an organised manner with a clear methodology. A methodology for developing ANN models was proposed by Wu et al. (2014). The steps proposed by Wu et al. have been modified into the following steps:

- Data Preparation
- Model Architecture Selection
- Model Structure Selection
- Model Calibration
- Model Validation
- Model Implementation

An overview of the number of articles considering these steps has been plotted in Figure 3. Note that articles can be counted multiple times if multiple steps have been considered. Articles have only been included in each section if clear recommendations were given on the specific modelling step.

Figure 3: Distribution of papers by modelling step considered.



3.1 DATA PREPARATION

Data preparation involves the processes of input selection and data splitting. Input is divided in to the procedure of selecting input parameters based on input significance and input independence (Bowden et al., 2005).

Input significance is the significance of the relationship between potential inputs and outputs. Techniques to assess this relationship are often analytical methods based on correlation and mutual information (Li et al., 2008). For some modelling exercises ad-hoc methods based on available data and/or domain knowledge have to be used. An iterative process can also be followed by applying constructive or pruning methods while calibrating the model (Diamantopoulou et al., 2007). Other popular methods are the use of genetic algorithms and trial-and-error (Maier et al., 2010).

Input independence is often not assessed but there are several methods to determine input independence. These methods can be divided into dimensionality reduction methods and filtering methods. Dimensionality reduction can be achieved by principal component analysis and clustering analysis or self-organising maps (SOM) (Maier et al., 2010, Cho et al., 2011). Filtering is similar to the pruning method in input significance where the partial mutual information is assessed (May et al., 2008).

Data splitting involves the splitting of the dataset into training, validation and test sets. Random data splitting is most common but sometimes an understanding of the underlying physical process or domain knowledge is taken into account (Haas, 2004). Sometimes predefined rules are set to the data sets to have an equal statistical distribution across all sets. This is often achieved by trial-and-error or optimisation methods like genetic algorithms (Maier et al., 2010).

An overview of the articles reviewed which discuss data preparation can be found in Table 1. Articles on general modelling have also been included as they add value to the overall goal of developing a model for water treatment plant performance.

Al-Abri & Hilal (2008) have used neural networks to model the coagulation and filtration process. They compared modelling results between raw data and data that has been transformed using principal component analysis (PCA). They have found PCA is generally good for reducing computation time at the cost of accuracy. Dürrenmatt & Gujer (2012) argue expert knowledge should be used to reduce datasets to meaningful and reliable sensors and use PCA to prevent collinearity between input parameters. They found applying PCA resulted in less accurate models which they account to the loss of information in applying PCA.

Baxter et al. (2001) used ANNs to describe a variety of variables within water treatment. They recommend the dataset should be representative for the full treatment window. At least a year of data is recommended due to the

Table 1: Details of papers reviewed including data preparation

Author	System	Modelled variable(s)
(Al-Abri & Hilal, 2008)	Drinking water (filtration)	Retention time and Fouling
(Baxter et al., 2001)	Drinking water	Colour, Flow demand, Particle count, Chemical doses
(Bowden et al., 2005)	General modelling	-
(Ding et al., 2014)	Drinking water	Water quality
(Dürrenmatt & Gujer, 2011)	Waste water	COD, Ammonia
(Griffiths & Andrews, 2011)	Drinking water (filtration)	Turbidity, Particle count
(Juntunen et al., 2012)	Drinking water	Aluminium and Turbidity
(Maier & Dandy, 2000)	General modelling	-
(Maier et al., 2010)	General modelling	-
(Mjalli et al., 2007)	Waste water	TSS, COD, BOD
(Baxter et al., 2002)	Drinking water	Turbidity
(Wu & Lo, 2010)	Drinking water	Coagulant dose
(Wu et al., 2014)	General modelling	-

cyclical nature and descriptive statistics could be used to identify daily or seasonal variations. Griffiths & Andrews (2011) go one step further in suggesting seasonal datasets should be used and a model for each season should be developed. Ding et al. (2004) also suggest categorisation might be beneficial for large datasets but at the cost of model accuracy.

Juntunen et al. (2012) used statistical methods to determine model inputs and reduce model complexity. Water processes, however, are often nonlinear systems which can't be fully captured by correlation coefficients and although Juntunen et al. found accurate correlations, critical information might be lost by not considering the nonlinearity. Wu & Lo (2010) also suggest selecting input parameters based on the correlation coefficient is sufficient. They found data normalisation doesn't have a significant effect.

Mjalli et al. (2007), however, argue data should be normalised to have zero mean and unity deviation. They argue it is therefore less likely for machine learning models to overfit or underfit. They had moderate success in modelling waste water treatment plant performance.

Smith et al. (2002) suggest single output models should be preferred over multiple output models to reduce the overall prediction error. They also suggest input selection should be based on known or suspected relationships, literature and data availability.

Bowden et al. (2005), Maier & Dandy (2000), Maier et al. (2010) and Wu et al. (2014) are not specific on water treatment but do provide a clear methodology on modelling. It provides a framework and guidance in the overall goal of modelling the performance of a water treatment plant.

3.2 MODEL ARCHITECTURE SELECTION

Model architecture selection involves the selection of the modelling method e.g. ANN, regression or genetic programming etc. The main architectures considered in this review are listed in Table 2.

Within ANNs several sub-architectures exist but the most common architecture is the multi-layer perceptron (MLP), which is a feedforward neural network consisting of an input layer, a number of hidden layers and an output layer. Other architectures may include feedback loops which enables the model to describe dynamic systems better (Wu et al., 2014, Karamouz et al., 2008).

Akinmolayan et al. (2005) investigated the use of mechanistic models within water treatment. They found mechanistic models to describe the overall trends moderately well but they were unable to describe specific events accurately making them less interesting for predictive modelling. Conlin et al. (1997) also investigated the use of mechanistic models and found that mechanistic models in combination with ANNs gave the best

Table 2: Several model architectures and descriptions in order of increasing complexity and decreasing transparency

Model architecture	Description
Least Squares Regression (LSR)	Least squares regression is based on the minimisation of the sum of squares between the data points and regression line. It is a simple model usually used when there are a small number of variables and where the relationships are linear or linear after transformation.
Genetic Programming	Genetic Programming is a modelling technique best represented by an evolving tree structure. Trees are built up constants, operators and variables resulting in a mathematically easy to understand relationship.
Support Vector Machines (SVM)	Support Vector Machines is one of many case-based reasoning methods but generally the most accurate. Data is classified in different classes and an output is linked to the class. Only useful when a lot of data is available and the whole range is captured.
Principal Component Regression (PCR)	Similar to LSR but the dimension of the input data is reduced.
Artificial Neural Network (ANN)	ANNs make use of hidden layers to transform the data, apply weights to the new layers and resulting in an output. ANNs are highly complex but are able to find accurate correlations.

performance. The use of hybrid models or combined models could have a beneficial effect.

Dürrenmatt & Gujer (2012) explored several types of architectures but found no significant difference in performance between these architectures. They suggest in that case selection should be based on secondary parameters like model transparency.

Hong Guo et al. (2015) compared ANNs and Support Vector Machines (SVMs) for the prediction of wastewater treatment plant (WWTP) effluent concentrations. Both models were able to describe effluent Total Nitrogen. The SVM performed better in accuracy while the ANN elucidated more on the physical related cause-and-effect relationship. Both were found suitable for prediction but the ANN describes the intrinsic relationship better. Juntunen et al. (2012) also compared two model architectures, the ANN and Least Squares Regression (LSR). They found the nonlinear ANN model was able to describe the process better but the improvement found was small compared to the results of LSR. They suggested a simpler model is used if the complex ANN does not improve model performance significantly.

Kennedy et al. (2015) investigated four different types of ANNs. Although they found the multi-layer perceptron to yield best results, they were unsuccessful in their secondary objective to determine which type of ANN model will provide best results beforehand.

Articles from Chunanbo Guo et al. (2015), Chau (2016), Gray & MacDonell (1997), Maier & Dandy (2000), Maier et al. (2010) and Wu et al. (2014) provide information on modelling in general and the differences between the architectures which is essential in the overall objective of modelling the performance of a water treatment plant. They provide guidelines and recommend domains in which to use which model architecture.

3.3 MODEL STRUCTURE SELECTION

Model structure selection is the determination of the number of layers, nodes, terms etc. and their interconnectivity. There are three main methods to determine the model structure (Maier et al., 2010). The first one is trial-and-error or past experiences. The model complexity is chosen and the performance evaluated after which adjustments to the model structure are made and the performance is evaluated again.

The second method includes constructive or pruning methods. These are stepwise model structure selections where the performance is evaluated after each iteration. A typical indicator of termination is the coefficient of determination (R^2) reaching a certain threshold or its change after each iteration not considered significant anymore.

Lastly, there are global optimisation methods which determine the best option within given bounds. These aren't commonly used due to the complexity involved.

Model structure selection is usually not discussed. Maier & Dandy (2010), Maier et al. (2010) and Wu et al. (2014) provide general guidelines on modelling as seen in the previous sections.

Al-Abri & Hilal (2008) and Smith et al. (2002) selected their model structure by trial-and-error with no clear methodology. Griffiths & Andrews (2011) also determined their model structure based on trial-and-error and found the optimum number of neurons to be 75% of the number of input parameters.

More focus should be given to the systematic approach of selecting model structure. Most of the articles don't mention their approach and although trial-and-error is a sound approach in most cases, it is not transparent and hard to reproduce the authors followed process for model structure selection.

3.4 MODEL CALIBRATION

Model calibration is the process of adjusting model parameters and forcing within the margins of uncertainties to obtain a model representation of the processes of interest that satisfies pre-agreed criteria.

Calibration methods can be either global or local. Most modelling methods use local calibration where in each iteration, the weight is changed slightly until it finds a minimum (which can be a local minimum). Global calibration adjusts the weights randomly and picks the minimal value found. There is less chance of finding a local minimum but global calibration is significantly more time consuming.

Model calibration is not a topic which is discussed in great detail. In the reviewed papers, it was most of the times inherent to the model used and therefore not discussed, hence the limited number of articles discussed in this section.

Maier & Dandy (2000), Maier et al. (2010) and Wu et al. (2014) offer guidance in model calibration selection while Zahrim et al. (2015) used response surface methods for model development. In principle there are only two main methods for model calibration and there is no best option as this will be dependent on the dataset. Maier et al. (2010) found that evaluation of the different calibration methods has had very little attention and is an area to be explored.

3.5 MODEL VALIDATION

The purpose of model validation is to exclude errors or detectable flaws from the developed model so it can be used for its intended purpose with confidence. Replicative, predictive and structural validity are the three aspects model validation should consider.

Replicative validity is inherently connected to model calibration as it is the evaluation of the trained model with data previously used in other steps of the model development. Replicative validity is often not checked as it is assumed the model calibration results are valid. Additionally, the error distribution could be explored to verify if there is a normal distribution.

Predictive validity tests the generalisation ability of the model by applying a new, unknown dataset to the model. This is usually evaluated by the validation and optionally the test dataset. Validity is evaluated with quantitative error measures like the coefficient of determination (R^2), Mean Absolute Error (MAE) and the Approximation Error.

Structural validity is the evaluation of the model outside of the bounds of the training dataset. This is usually done by a sensitivity analysis and evaluating if the outcome is plausible and follows expectations. It is also a method to determine the uncertainty of the model.

Gontarski & Rodrigues (2000) argue validation should be used to determine the input parameters in an iterative process to improve the model efficiency. Whereas it would be ideal to be able to predetermine the input significance, it is important to improve the efficiency when creating a holistic water treatment plant model comprising several unit models.

Griffiths & Andrews (2011) suggest using the MAE and R^2 as indicators for predictive validity. As the MAE is not normalised, when evaluating different models with different ranges a better metric would be the Approximation Error which is a relative error measure. Rak (2013) on the other hand suggest the correlation coefficient is an important indicator. This may be true for predicting overall trends but not for accurate modelling of performance.

Hong Guo et al. (2015) conducted a sensitivity analysis to evaluate structural validity. They compared two models which performed equally well but surprisingly had a significant difference in significant input parameters. In combination with the sensitivity analysis this indicated the input parameters weren't independent and they suggested in this case input selection should be re-evaluated.

Kennedy et al. (2015) compared several models which had similar performance. They suggest additional metrics should be used when there's no apparent preferred model. Secondary metrics like model transparency, efficiency and others should be important in selecting the preferred model then.

Smith et al. (2002) suggested replicative and predictive validity should be evaluated by rearranging the datasets. This enables evaluation of the stability of the model. Yoon et al. (2011) suggests evaluation of the model should be done by evaluating the generalisation ability in the form of ratio tests between the root-mean square error (RMSE) of the test and train set and the validation and train set. A value close to 1 for both ratios would be the perfect case indicating the model has not overfitted or underfitted for a specific dataset.

Maier & Dandy (2000), Maier et al. (2010) and Wu et al. (2014) again provide general modelling guidelines.

3.6 MODEL IMPLEMENTATION

After unit models have been created and validated they have to be combined into one model. One step further could be the implementation of the model into the plants control system. Articles on model implementation in the water treatment industry are quite limited. There is, however, enough literature available about model implementation in other industries.

Dürrenmatt & Gujer (2012) argue the importance of implementing some measure of uncertainty when implementing model based parameters into a control system. Although it is important to know there is a measure of uncertainty it can be argued this will not improve plant performance and might actually make the industry more reluctant to model implementation in control systems.

Griffiths & Andrews (2011) suggest a model for implementation should be run alongside actual operation to evaluate current capabilities. Smith et al. (2002) argue that the model is only valid as long as the input parameters stay within the calibrated range and the model requires updating when values are out of range. Zhang & Stanley (1999) go one step further in suggesting real-time learning should be implemented for continuous model improvement. Maier (2004) warns for scaling issues when implementing the model at a full scale plant.

4 DISCUSSION

Although the number of relevant articles are limited some valuable information has been gained. The topic of traditional modelling methods in water treatment will be discussed after which the implementation of ANNs will be discussed. The discussion will be concluded with the applicability to a complete predictive water treatment plant model.

4.1 TRADITIONAL MODELLING METHODS

Traditional modelling methods have limited applications as most of the methods are unable to describe the complex nonlinear relationships that exist in water treatment. One of the most accepted models nowadays is the surrogate for organics: UV absorbance at 254 nm (Korshin et al., 1997). Most other parameters, if not all parameters, used in plant control are directly measurable. A lot of plants still rely on lab sampling for process control which is time consuming and has a lag factor. Lab samples have been established and the confidence level in the results are high in contrast to models which carry an inherent error measure and values cannot be verified easily.

The major flaw in traditional modelling methods is the inability to describe complex nonlinear problems accurately. Although academics have come up with theories on water treatment processes, the models are able to describe the process in general trends but are unable to describe them in detail and in specific events. A model is usually developed to get a better understanding of the process and to help in determining areas of improvement and developing contingency plans in a cheap and effective manner. This makes these models unsuitable for plant control or planning purposes.

Despite the known flaws several processes can sometimes be described by linear models and where possible this should be implemented as linear models usually are transparent, easy to understand and easy to adjust or recalibrate. They are computationally more efficient so they should be implemented where possible.

4.2 ARTIFICIAL NEURAL NETWORKS

The use of artificial networks in plant control or for resource planning in water treatment is very limited. A few articles, like Griffiths & Andrews (2011), mention implementation of artificial neural network models in the plant control system, but they are run in parallel and are not actually part of the control system. Models will always carry a certain amount of risk and error but this is no different from lab sampling for instance. It is, however, the inability to verify the error what makes ANN models implemented in plant control systems limited.

There are endless possibilities for the use of ANNs in water treatment. The performance and accuracy is, however, very much dependent on the quality of the dataset and the chosen model structure. A key risk in ANN development is overfitting or underfitting the data. Generalisation of the model is very important but is hard to

quantify. Yoon et al. (2011) have already suggested evaluation of the generalisation ability could be done by determining the ratio between the RMSE of the different datasets. Generalisation could also be assessed by conducting a sensitivity analysis on the model and evaluate the results of extreme but plausible input values. The generalisation ability of a model is not often discussed in literature and is a subject which should receive more attention.

The main drawback of developing models using ANNs in the water treatment industry is the fact that each plant is unique and the created models are, in most cases, non-transferable. This makes modelling of performance both costly and time consuming. A point of focus in the future should therefore be investigating the possibility to normalise and generalise data to enable models to be transferable. This is an inherent flaw of ANNs and most other modelling methods that it is an empiric approach and the model is only as good as the input data. Nevertheless, efforts could be made to normalise input data for local dimensions. For instance, by using solids load for filters as an input instead of flow, turbidity and physical filter parameters like surface area and depth.

ANNs are very promising and should be used more often in industry but caution is advised to what the model is actually describing and what the error is. If proven to be successful it can be a powerful tool in creating accurate models.

4.3 PREDICTIVE WATER TREATMENT PLANT MODEL

Constructing a complete predictive water treatment plant model is a difficult process. All models will carry a certain amount of error, which, when put in series, can have major consequences. On the other hand, a complete predictive water treatment plant model could be used to understand plant performance under adverse water quality conditions and may therefore be a tool to determine bottleneck(s) and may help in capex decision making. In general, it could also be a tool to determine how the plant should be run to maximise efficiency. When used for decision making the model has to be accurate, generalised and fit for purpose.

In order for a model to be fit for purpose it should be made as simple as possible. The amount of building blocks should be kept to a minimum to minimise the evolving error. The same goes for the number of parameters used as these could contribute to the error. In the authors view it is therefore important to evaluate input significance and independence.

Another subject that should receive more attention is the generalisation of the models used. If possible, models should be built in such a way that when upgrade work is done, the model can be adjusted easily by changing several constants. On the other hand, this could also help in the validation and confidence in the model by assessing the model on a different plant with similar treatment steps.

The implementation of ANNs or any other model type in the creation of a predictive water treatment plant model is an area which hasn't been explored extensively yet and a lot of risks exist in doing so. Nevertheless, with the current state of modelling methods and computing power it is possible to create very accurate models. Caution should be taken when assembling the building blocks and a lot of care should be taken when selecting the input parameters.

5 CONCLUSION

Published work on modelling water treatment plant performance is very limited. Although a larger number of articles are published than reviewed in this paper, a lot of articles are factual statements and lack discussion to help future modelling endeavours.

Many papers highlight the data preparation step. A model is only as good as the dataset and plays a crucial role in achieving your modelling goals. Several methods are used to divide datasets but more attention should be given to selection of inputs based on significance and independence. Including too many parameters may result in overfitting the model and increasing the error function while including too few parameters may result in underfitting and not capturing the true relationship.

The model structure and architecture selection is usually done at the project start and only a few papers evaluated the performance of different model types. The more traditional modelling methods have a clear deficit

to ANNs in their ability to describe nonlinear problems. Nevertheless, these models should still be explored as they are more transparent and therefore easier to use when creating an overall predictive water treatment plant model.

According to Maier et al. (2010) over 60% of the model structure selections is done ad-hoc. A more systematic approach in the form of a stepwise pruning or constructive method would improve the justification for a certain chosen model structure. Justification of decisions made is a feature often lacking in papers.

Model calibration is a topic rarely discussed in the literature. The calibration method is usually connected to the chosen model architecture but within ANNs several calibration methods exist. It can be concluded that in most articles the model has been calibrated locally. If the error surface is smooth this is the most efficient method in finding the best correlation but this is not always the case. Unfortunately, there hasn't been much research on the evaluation of different calibration methods and this is an area that should be investigated further.

Model validation is usually done by evaluating the performance with statistic parameters. This gives a good indication on the validation of the model on the dataset but more extensive validation should be explored more often. Structural validity should be tested by conducting a sensitivity analysis and even predictive validity should be evaluated more by assessing the generalisation ability.

Model implementation is rarely reported but the general consensus is to have extensive testing by running the model alongside plant operation. Performance of the model can then be evaluated and changes could be made based on new findings. This area hasn't been explored much yet and methodologies aren't yet developed for the water treatment industry.

Overall a lot of insights have been gained on modelling in the water treatment industry and valuable lessons and tips have been gathered which help in developing a water treatment plant model. Two areas have been identified as important: data preparation in the form of input selection and model validation by assessing the generalisation ability.

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