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Neural network modelling and prediction of an Anaerobic Filter Membrane Bioreactor

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ABSTRACT

Anaerobic membrane bioreactors have become an environmentally friendly solution for wastewater treatment. The lack of sufficiently accurate mathematical procedures to model their behaviour and the fouling process of the membranes, poses a challenge when trying to optimise their energy consumption and maintenance costs. An accurate model of the fouling process of the membranes is critical to make the most of this technology. This is a perfect scenario in which to introduce neural networks (NN) as an alternative to mathematical modelling. However, the duration of the experiments and the difficulties in measuring some relevant variables, make it hard to collect high quality datasets to train the NN. Our goal is to obtain a good prediction of the fouling status of the membranes to enable an adjustment of operation conditions and maintenance procedures ahead in time. To do so we must obtain high quality datasets to train our neural networks. The combination of static and dynamic networks enables us to leverage the best prediction capabilities of each one. This combination requires a preprocessing of the datasets that separates trends from oscillations. The outputs obtained need to be put together to build up the predicted evolution of fouling. Accurate predictions are then extended from 25 to up to 75 filtration cycles. To maintain and even extend accuracy after sudden changes in operating conditions, retraining the NN every 25 cycles is proposed. AI based real time predictions open a new scope for decision making, and optimisation in the field of anaerobic membrane reactors.

1. Introduction

Anaerobic membrane bioreactors (AnMBR) combine anaerobic digestion along with membrane technology to provide an efficient treatment of wastewater with energy recovery as biogas. Their applications range from low concentrated domestic effluents to high concentrated industrial wastewater. One of the key factors affecting their technical and economic viability is the filtration capacity of the membranes, which is reduced by fouling (Judd, 2011). Fouling is a complex problem, affected by multiple factors, including wastewater characteristics, membrane and biomass properties, and operational conditions such as filtration flux and duration, backwash frequency, flux and duration or gas sparging for membrane scouring and their mutual combination (Martínez et al., 2021).

Our goal is to extend membrane life and reduce maintenance costs by modifying operating conditions to prevent high irreversible fouling before it develops. Previous studies expose the lack of reliable mathematical models to relate operating conditions to membrane fouling (Ludwig et al., 2012; Villarroel et al., 2013). Response surface methodology (RSM) has been used to investigate the effect of multiple operating conditions of the bioreactor on a response variable, generally the membrane fouling rate (Martínez et al., 2021). Artificial intelligence has revealed as a viable solution to analyse the relationships between different influential parameters and membrane status. Many studies have been conducted on this area as summarised in Bagheri et al. (2019). Irfan et al. (2022) compared membrane permeability predictions obtained with RSM and feed forward neural networks, checking that AI provided higher accuracy. Neural networks have been applied in other water management related areas as well (Ostad-Ali-Askari et al., 2017). Nevertheless, these relations do not offer enough information for decision making. To prevent membrane fouling and therefore modify operation settings of the plant, some sort of anticipation is required. Fouling prediction has not received much attention in literature so far. A recent work (Nam et al., 2021) has tackled this issue. Using state of the art artificial intelligence and machine learning techniques, the authors predicted the behaviour of relevant parameters affecting membrane fouling. These parameters were taken as inputs for an integrated MBR model. This allowed the authors to make accurate predictions one day ahead. Our final goal is similar to theirs, although we avoid the use of mathematical models and rely uniquely on artificial intelligence solutions to relate inputs and outputs.

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This work will demonstrate that this approach is feasible, yet not simple. Most of its success is based on the quality of the datasets collected and the pre-processing of the information before entering the neural network training process. One day ahead prediction is an ambitious objective and will not be directly achieved but, by means of a periodic retraining process, the necessary anticipation can be obtained.

The novelty of this work resides mainly in four aspects. Firstly, the use of a broad dataset of membrane fouling to ensure the best possible training of the neural networks. Data of membrane fouling include flux and transmembrane pressure collected every two seconds and hydraulic resistance and, particularly, reversible fouling rate processed to obtain input and output values for each cycle for hundreds of operation cycles. Secondly, the combination of two different neural network technologies, Feed Forward Neural Network and Long Short Term Memory, to leverage the best prediction capabilities of each one. Thirdly, the preprocessing of the dataset via a digital filter to feed each network with the most adequate information. As a result, the prediction of the fouling status of the membrane hours before a critical condition is reached, to allow maintenance procedures and operating conditions to be adjusted and extend membrane's life.

The rest of the paper is organised as follows:

- Related work: a review of previous work by researchers in this field is presented. It is mainly focused on the solutions proposed for wastewater treatment plants and, more specifically, on the application of Artificial Intelligence and Machine Learning techniques on membrane fouling processes.
- Materials and methods: the experimental framework on which this work has been based is described. Data selection, modelling and prediction decisions are also presented. The use of digital filters on data preprocessing is explained.
- Results and discussion: in this section the results obtained in this work are presented, along with a discussion on how satisfactory they are and how retraining can improve real time decision making.
- Conclusions: the main achievements of the paper are detailed along with an introduction to future research lines in this area.

2. Related work

Intensive research has been conducted on how to control the fouling processes, aiming to minimise maintenance works and maximise membrane lifespan. Mathematical fouling-process models were applied to the optimisation of operating conditions of membrane bioreactors. Li and mao Wang (2006) developed a mathematical model to determine the pressure increase on the basis of filtrated volume per unit of area, using a potential equation of the main operating variables: filtration flux, aeration intensity, sludge concentration, and sludge stickiness. The model parameters were selected based on laboratory tests but also on previous reported data and some other assumptions. The simulated results showed that membrane fouling was mainly affected by filtration flux, followed by aeration intensity and sludge concentration. Wu et al. (2012) modified the aforementioned model, to include the effect of colloidal and soluble components and solids of different floc size distribution. This revealed a detailed cake structure, including the spatial distribution of cake porosity, the specific cake resistance, and the synergistic interactions among major fouling factors. The main limitation of these models for their widespread application is the calibration of model parameters, including the density of deposited soluble, colloidal components and suspended solids within the layer, as well as online analysis of particle size distribution for real-time prediction of membrane fouling. This has led researchers to find alternative approaches. Neural networks have already been explored in literature with uneven results.

Soleimani et al. (2013) propose a model of a filtration unit for oily wastewater based on ultrafiltration membranes. Using trans-membrane pressure (TMP), cross-flow velocity (CFV), feed temperature and pH as inputs, the model produces values of permeation flux and fouling resistance as outputs, using a multilayer perceptron training on a dataset composed of input/output combinations measures over the course of 2.5 h. During this short period of time, the membrane state is considered steady. In this condition, the static neural network proposed produces very accurate outputs as a response to inputs within the bounds of the training dataset.

Mirbagheri et al. (2015a) simulate transmembrane pressure and permeability as functions of: time, total suspended solids (TSS), chemical oxygen demand (COD), solids retention time (SRT) and mixed liquor suspended solids (MLSS). They use two types of forward neural networks with one hidden layer in both cases. What is most relevant as a precedent to our present work is that time is considered as an input. Unlike (Soleimani et al., 2013) the authors collected data over the course of 60 days, a period of time way too long to assume that the membranes are in a steady state. Time reflects the progressive fouling of the membranes; without time in the equation, the same input parameters may produce different output values, thus making the training process unfeasible. In Mirbagheri et al. (2015a), two consecutive working regimes are considered: conditions during the first half of the time taken for the experiments differ drastically from those in the second half.

Hazrati et al. (2017) introduces the use of neural networks to model COD and TMP as a function of hydraulic retention time (HRT) over the course of several months. HRT took three different values, leading to three consecutive working regimes. TMP grew steadily over time despite of the regime, but, COD dropped significantly on each shift on HRT. Despite these drops on HRT, the authors stick to time as a representation of the membrane's current state and the model works fine.

Unlike the already mentioned precedents, Geißler et al. (2005), relies on a recurrent neural network to model permeate flux on a submerged membrane bioreactor. The Elman network takes into consideration its current state along with the input values to produce its prediction. This behaviour considers the passage of time to improve predictions trying to reflect the influence of the system's recent history on the coming outputs. Filtration and backwash times are also taken as input values. Nevertheless, the authors took hourly averages of all inputs to train the network which, depending on the length of the filtration cycle, may have produced some oscillation in the data. More recently, Woo et al. (2022) show how AI can be used to predict membrane's lifetime over long periods of time.

Bagheri et al. (2019) presented a review of all what, to that date, had been done around Artificial Intelligence applied to membrane fouling in filtration systems. The authors classify previous work according to different concepts: modelling, simulation and prediction. Although not mentioned among their classificatory factors, optimisation is also present in the review.

The three major areas where Artificial Intelligence may be applied to these filtration systems are:

- Modelling: creation of a model of a certain filtration system to reproduce, accurately enough, system's behaviour under several different operating conditions. Modelling facilitates the analysis of the underlying mechanisms of the filtration system. The internal dependencies, weights in the case of neural networks, may reveal interesting actual dependencies within the AnMBR plant under scrutiny. Modelling enables system simulation as an alternative to real testing thus reducing testing times from hours/weeks to seconds/minutes. This concept includes both modelling and simulation concepts used in Bagheri et al. (2019). Several AI based techniques for fouling modelling are compared in Hamedi et al. (2019). In this study, temperature, permeate flux mixed liquid suspended solid and transmembrane pressure are taken as input parameters. The authors concluded that LSSVM models outperform other techniques such as MLP. Similarly Radial Basis

Function Neural Networks have been explored in other studies (Mahmod and Wahab, 2017; Mirbagheri et al., 2015b) as an alternative to FFNN, yielding even better accuracy. Although not common in this field, some other applications introduce different algorithms to determine the optimal number of neurons (Giwa et al., 2016) or to replace back propagation in FFNN training. Genetic Algorithms are a popular solution (Montana et al., 1989), but more recently other interesting alternatives have been explored: optimal foraging and marine technology are explored in Ho et al. (2021), an antlion optimiser is introduced in Ho et al. (2022) and balancing composite motion optimisation is applied in Khatir et al. (2021), among others. In many cases, the extra computational complexity these techniques introduce, is offset by the quality of training. Modelling may also be used, not to reproduce membrane's performance, but to investigate the relative influence of different input parameters on this behaviour (Schmitt et al., 2018).

- Prediction: in Bagheri et al. (2019) static neural networks such as the multilayer perceptron, used to generate output values produced by input values that are within the training intervals, are referred to as "predictive". This definition of prediction, although common in literature, does not anticipate response values ahead in the future.
- Optimisation: this concept entails the use of a previously generated model of the actual system to feed an optimisation algorithm in search of the best settings to obtain a certain response. Soleimani et al. (2013) implemented a multi-objective optimisation procedure based on genetic algorithms to maximise permeation flux and minimise fouling resistance.

Zhao et al. (2020) review the application of artificial intelligence and machine learning to wastewater treatment and provides a classification of the technologies applied to the different processes involved. This study revealed that different approaches have been adopted by different authors so the best technique to be applied is still an open question. Previous attempts to predict the future behaviour of filtration membranes are presented in Shi et al. (2021); authors present a comparison between AI based procedures, mathematical and mechanism analysis. They conclude that future research should address membrane's remaining useful life prediction. A more recent review from Kamali et al. (2021) focuses on membrane fouling processes and concludes that *"AI methodologies have not yet been employed for the monitoring and control of membranes for water and wastewater treatments specifically in case of MBRs"*. Nevertheless, almost simultaneously to this statement, Nam et al. (2021) introduces a novel methodology to obtain predictions over membrane behaviour and apply them to make real time decisions meant to decrease fouling and increase efficiency. So far, both static and recurrent neural networks have been tested. Input parameters are time, TSS, COD, pH, SRT, HRT, MLSS, CFV, TMP, backwash transmembrane pressure (TMP_{bw}), reversible fouling rate as increase in TMP over time (dTMP/dt), temperature and oxygen decay in the aerobic zone. Output values were: TMP, permeation flux, COD removal and fouling resistance. It is important to note that operating conditions such as the duration of filtration cycle (t_c) and the duration of backwash cycle (t_{bw}) are not present in most of the studies. However, authors often search for relationships between physical parameters as AlSawaftah et al. (2021) expose. The control over the membranes demanded by Kamali et al. (2021) can only be obtained if operating conditions are part of the equation. They can be altered as a consequence of the observed and predicted output parameters such as fouling resistance. Literature tends to merge the concepts of "modelling" and "prediction", assuming that the accuracy of the neural network measured over the training data set implies that a good model of the process has been obtained and can be applied to predict future responses. Even though, input variables can be kept within the values taken during training, the very passage of time leads to different response values in the future.

The use of neural networks to enhance the accuracy of alternative models has been applied to many other fields. State of charge (SOC) determination on batteries is one of them. Jiao et al. (2021) introduce different, and a-priori more precise, mechanisms to determine the status of a battery and expose their its flaws. Then a neural network-based methodology is proposed. Similarly to our process, relationships between physical parameters change over time and need to be taken into account to produce accurate results.

This work has two major objectives:

- To obtain an accurate model of the filtration tank of an AnMBR pilot plant.
- To extend the model to make predictions beyond the training set in order to anticipate maintenance procedures on the membranes. Different types of neural networks, along with data pre-processing techniques not previously applied in this field, will be explored in order to anticipate plant's response as much as possible.

3. Materials and methods

3.1. AnMBR pilot plant

The AnMBR used in this work Fig. 1 was installed in the Campofrio Frescos slaughterhouse (Campofrio Food Group, Burgos, Spain) It consisted of a down-flow anaerobic filter filled with plastic carriers (Biofill-C, Bio-fil) for biomass immobilisation, and an up-flow filtration tank where a submerged hollow fibre membrane (Zenon Zeweed-10) was placed. Anaerobic filter and filtration tanks were connected at the bottom and at upper parts for mixed liquor recirculation. Diaphragm compressors (Secoh SV50) were used for gas sparging, for membrane scouring and gas-lift recirculation. A reversible wear pump (Micropump Eagle Drive GJ-N21) was used for filtration and backwashing. Temperature of biological process was kept at 30±1.0 °C by means of an electric heating blanket. Pressure sensors (PN 2569, IFM) monitored transmembrane pressure, and filtration and backwashing flux were measured using inductive flow-meters (MIK 5NA, Kobold Mesura). Temperature (TR2432, IFM), pH (Liquiline CM14, Endress+Hausser) and biogas production (FCI ST75) were continuously monitored. The slaughterhouse wastewater was characterised by oil and grease (O&G) concentrations between 830 and 960 mg/L, COD and Total Organic Carbon (TOC) concentrations of 2530–5210 mg/L and 1150–2030 mg/L, and Total Nitrogen (TKN) of 830 960 mg/L. The bioreactor was previously operated as internal gas-lift reactor treating slaughterhouse wastewater during 4 months.

Our plant is integrated by an AnMBR experimental reactor comprising a biological reactor and a filtration tank with a volume of 0.016 m^3 with a submerged hollow fibre membrane (Zenon Zeweed-10) with pore size 0.04 μm and filtration area of 0.93 m^2. A diaphragm compressor was used for membrane scouring by biogas recirculation, and a reversible wear pump was used for filtration and backwashing. A detailed description of the AnMBR pilot plant can be found in Diez et al. (2018). The filtration unit is what we aim to model by means of a neural network.

3.2. Monitoring and control

Pressure sensors, liquid and gas flowmeters, temperature and pH-meters were used for the AnMBR monitoring. An Arduino based PLC is used to monitor and control the whole system. This is a low-cost automation solution capable of operating the plant and to providing real time information on its performance. Information is serially conveyed to a local PC for all time analysis and monitoring. The desktop application (Fig. 2) created for this purpose also features also command capabilities. The operations described ion this paper are based on the data collected by this application. Our desktop application has been programmed in Visual Basic.net language and features pre-processing, storage and both local and remote monitoring and command capabilities.

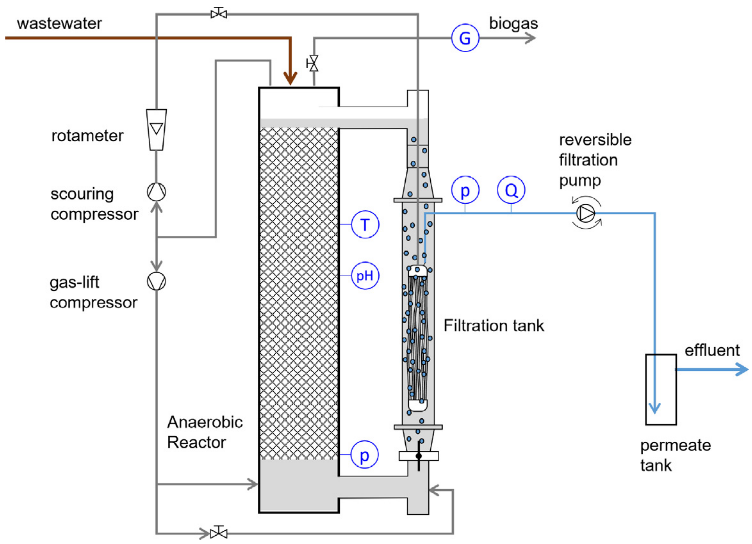


Fig. 1. Schematic diagram of the jet loop Anaerobic Filter Membrane Bioreactor.

Fig. 2. Desktop application main screen.

3.3. Data selection

Three major factors determine the success of a neural network-based model:

- The input and output parameters selected, though mainly the input ones since results are usually determined by the objectives of the model itself.
- The extent and representativity of the training dataset.
- The type and internal structure of the network itself.

As stated before, there are several parameters expected to influence membrane behaviour. Ideally, all those that produce a significant impact should be considered. However, there are certain parameters that are hard to obtain from the process in real time or even hard to measure at all. Some previous researchers chose not to neglect this information and decided to take samples at certain times, but this procedure tends to ignore relevant information about the process that is produced in between. This leads to a poor training data set, which in turn compromises the accuracy of the model. Moreover, our goal is to make dynamic predictions on how membranes are going to behave in the future. This makes the use of easily measurable parameters mandatory. Based on these constraints, the four following parameters were chosen:

- Filtration time or cycle time (t_c).
- Backwash time (t_{bw}).
- Filtration flux (J).
- Backwash flux (J_{bw}).

We are aware that, among other input parameters that may influence the behaviour of the filtration unit, the concentration of solids is particularly relevant. However, it cannot be measured during operation so this parameter must be excluded.

When the status of membranes cannot be considered steady over time, time itself can be taken as an input value. However, we choose to take the overall volume of filtrated water as the value responsible for changes in the filtration capacity of the membranes.

Output values are meant to represent the filtration capacity of the membranes. These are:

- TMP_0: transmembrane pressure at the beginning of the filtration period.
- dTMP/dt: TMP variation over time.
- R_0: hydraulic resistance at the beginning of the filtration period.
- dR/dt: R variation over time.

Transmembrane pressure TMP (Pa) was calculated according to Martínez et al. (2020).

Real time operation involves, not only sending and receiving data, but also its analysis. To do so, a set of mathematical methods was added to the program. The most relevant of all was the implementation of a robust regression function that converts each filtration/backwash cycle into a slope-intercept pair that represents the evolution of performance

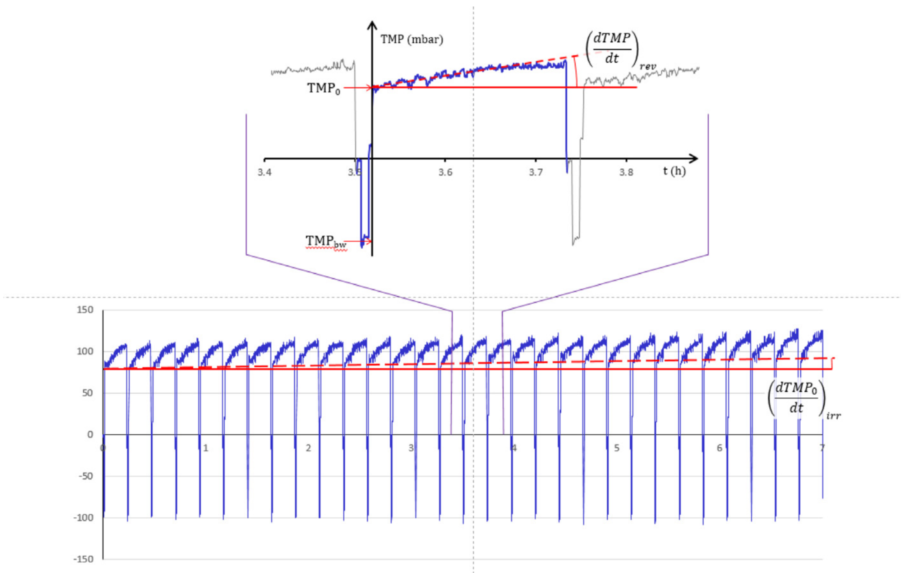


Fig. 3. Typical transmembrane pressure profile where TMP at the backwash and at the beginning of filtration, reversible and irreversible fouling are detailed.

for further analysis such as the neural network training and testing. Samples are taken every two seconds by the PLC and sent to the PC to perform these calculations in real time.

Fig. 3 shows typical TMP profiles. TMP_{bw} represents transmembrane pressure during backwash step. Weakly attached materials that can be removed by relaxation and backwash determine the reversible fouling rate $(dTMP/dt)_{rev}$, whereas materials firmly attached to the membrane that can be removed only by chemical cleaning are responsible for the irreversible fouling rate $(dTMP_0/dt)_{irr}$.

TMP_0, $(dTMP/dt)_{rev}$ and $(dTMP_0/dt)_{irr}$ were determined by robust regressions by the Huber method to avoid the leverage of the minimum squares linear regression method due to anomalous data associated to bubbling and vibrations. A Huber tuning constant of 1.345 was used according to 95% asymptotic efficiency rule.

Darcy's law (Darcy, 1856) was used to determine the hydraulic resistance at the start of the filtration period, R_0 (m^{-1}), Eq. (1), and to calculate the reversible fouling rate on resistance basis $(dR/dt)_{rev}$, Eq. (2) (Martínez et al., 2021):

$$R_0 = \frac{TMP_0}{\mu \bullet J} \tag{1}$$

$$\left(\frac{dR}{dt}\right)_{rev} = \left(\frac{dTMP}{dt}\right)_{rev} \frac{1}{\mu \bullet J} \tag{2}$$

were, J is the filtration flux ($m^3\ m^{-2}\ s^{-1}$) and μ the permeate viscosity (kg $s^{-1}\ m^{-1}$).

Our desktop application performs all the calculations. The calculated values of TMP_0, R_0, $dTMP_0/dt$ and dR_0/dt take the shape displayed in Fig. 4.

3.4. Modelling

When no algorithmic model has been found, neural networks can provide a good approach to describe the behaviour of the system. Still, finding out the most suitable type of network and its optimal design usually demands a significant effort. Thankfully, literature has already explored this field so we can find meaningful hints for a good start.

Modelling of membrane bioreactors has been largely studied to quite a large extent. Most previous workers agree that Feed-forward Neural Networks can provide a good solution. The training dataset plays an important role in the success of the resulting model. There are several ways to determine both the number of hidden layers and the number of neurons per layer. Some authors have employed heuristic methods such as genetic algorithms to find suboptimal configurations of this structure. Most authors, though, rely on trial and error procedures for this purpose. In this work, the latter approach has been followed, based on a broad training dataset obtained from many previous experiments conducted on the plant. A feed-forward back-propagation multilayer network was finally selected. The computational complexity of these and other networks has already been studied (Orponen, 2000). The network has two hidden layers integrated by 14 neurons each (Fig. 5). Matlab Deep Learning Toolbox was used for all the simulations performed in this work. Table 1 describes the most relevant parameters related to network training.

Table 1
Neural network training parameters used in this work for the simulations (with Matlab Deep Learning Toolbox).

Parameter	Value
Training epochs	up to 2000
Trainratio	0.70
Validation ratio	0.15
Test ratio	0.15
Data division	random
Training	Bayesian Regularisation
Performance	Mean Square Error

Table 2 shows the most relevant performance parameters of the networks when modelling the four outputs which we need to consider: R^2 (Coefficient of determination), MSE (Mean Squared Error), RMSE (Root Mean Squared Error), MAE (Mean Absolute Error), MAPE (Mean Absolute Percent Error), SD (Standard Deviation) and EV (Explanatory Variable) score. The number of training epochs and the time taken to complete them all are also provided. These results are among the best obtained by previous authors, even though the computational complexity of the model has been kept low. Values of R^2 (0.991) are well above those obtained by (Hamedi et al., 2019) from ANN-MLP models (0.5833) and as good as those obtained from LSSVM models (0.99).

3.5. Fouling profile prediction

The second objective proposed in this work involves predictions of the behaviour of the plant ahead in time. This is hard to achieve by means of a feed forward network since we must assume future response depends on the recent history of the filtration process. For these types of applications, recurrent neural networks offer more promise.

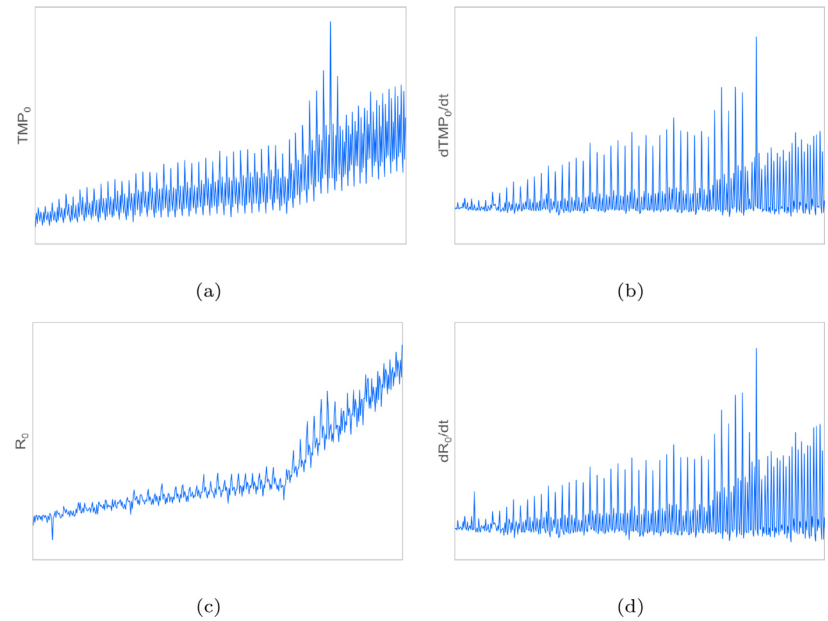


Fig. 4. Experimental patterns of TMP_0 (a), $dTMP_0/dt$ (b), R_0 (c) and dR_0/dt (d) vs cycle.

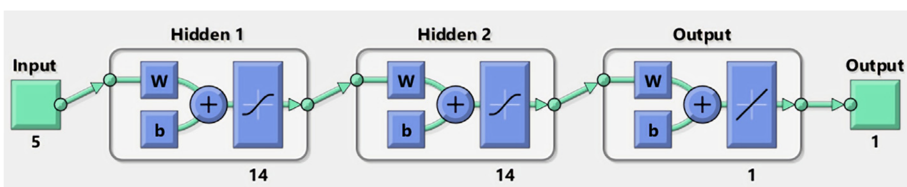


Fig. 5. Feedforward, backpropagation 2 layer network.

Table 2
Performance metrics of our model: R^2, MSE, RMSE, MAE, MAPE, SD and EV.

Output/Parameter	R^2	MSE	RMSE	MAE	MAPE	SD	EV	Epochs	Time (s)
R_0	0.9910	0.016	0.1030	0.0398	0.0205	0.1031	0.9910	835	15
TMP_0	0.9946	6.5973	2.5685	0.8571	0.0169	2.5678	0.9946	700	12
dR_0/dt	0.9671	0,00029295	0.0171	0.0052	0.5787	0.0148	0.9674	958	18
$dTMP_0/dt$	0.9286	0,9380	0.9685	0.1722	1.0134	0.9686	0.9287	820	15

Predictions are the second goal of this work. This objective entails two approaches:

- Short-term predictions.
- Mid-term predictions.

A good model of our filtration unit enables us to predict its response when working settings are changed. This is useful for several purposes among which is the search for optimal filtration and backwash times. However, our principal aim is to predict how the filtration unit will behave later in time. By doing so, we will be able to anticipate when the plant will need to undergo maintenance procedures. This upcoming behaviour will strongly depend on the previous sequence of input/output data already collected.

Recurrent networks are expected to somehow keep track of previous events and apply this knowledge to predict the upcoming ones. Among the numerous types or neural recurrent networks available, both the literature and our early tests determine that the most suitable ones for our purpose are Long–Short Term Memory (LSTM) networks. LSTM networks are a type of neural networks used for time series forecasting, that is, future states of an output can be predicted based upon the past values of inputs and outputs. Their ability to predict future events is discussed by Petneházi (2019).

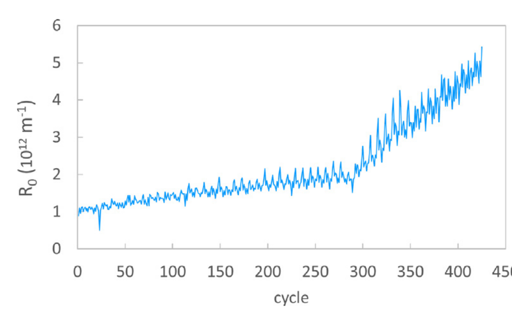


Fig. 6. Evolution of R_0 over 425 filtration cycles.

It is noted that LSTM networks are known to have difficulties when dealing with either periodic or trending data. A typical behaviour is depicted in Fig. 6 where real data representing the evolution of R_0 over time is shown. R_0 tends to increase in the long term but showing significant oscillations in the short term.

This behaviour is hard to anticipate as our early attempts soon revealed. The solution proposed to deal with this problem is to split the data set in two, separating the general trend from the oscillations

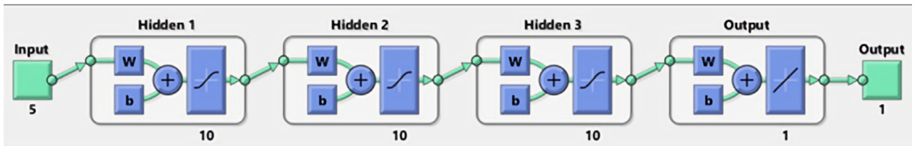


Fig. 7. Feedforward, backpropagation 3 layer network.

which involves some sort of filtering. The rest of the process will take the following steps:

1. Separate the trend from the oscillations in the output data series.
2. Predict their evolution separately: the trending part will be predicted by a static network, whereas the oscillating part will undergo a dynamic prediction.
3. Sum up the two results.

Zhang and Qi (2005) studied the need for deseasonalization and detrending datasets before making predictions based on artificial neural networks. We do not experience seasonality in our patterns but certainly trending is an issue.

Yi et al. (2019) propose data separation to extract trends from time series data. Trend separation is performed by linearisation of different stretches of the input data. Then prediction on trend and difference data are performed by means of a simple recurrent neural network (RNN) in both cases. We have also tried these types of networks but, the results obtained were not as good as those presented in this work. That said, for our input data, this linearisation procedure would be unsuitable since it would be too hard to know in advance how many stretches we should consider or how long they should be.

From the experience of numerous trials conducted before those we are about to present, the volume of water filtrated was not relevant for the training process of this dynamic network. It was the same for the rest of the input parameters for the static one. We thus used cycle times and flow rates to train the dynamic network, and only volume of water filtrated to train the static one.

The two hidden layer network used for modelling did not yield so good results for prediction. A slightly more complex three hidden layer feed forward network with 10 neurons on each layer was used for static prediction (Fig. 7). The rest of training parameters are still those presented in Table 1.

The dynamic prediction is performed by an LSTM network whose internal structure is the following. We paste the original Matlab code for any interested reader:

```
layers = [ ...
  sequenceInputLayer(featureDimension)
   lstmLayer(numHiddenUnits1,'OutputMode','sequence')
  fullyConnectedLayer(250)
  dropoutLayer(0.0)
  fullyConnectedLayer(numResponses)
  regressionLayer];
```

Training settings are:

```
options = trainingOptions('adam', ...
  'MaxEpochs',maxEpochs, ...
  'MiniBatchSize',miniBatchSize, ...
  'InitialLearnRate',0.0005, ...
  'GradientThreshold',1, ...
  'Shuffle','never', ...
  'Plots','training-progress',...
  'Verbose',0);
```

Less complex networks do the job in many cases but, to make results comparable, we keep the same settings in all prediction experiments. Training times are much longer on the LSTM network so, it is recommendable to simplify its structure when possible. The number of samples highly influences training times too.

3.6. Preprocessing

Raw data obtained from the process has undergone two pre-processing processes before entering the modelling and prediction stages:

1. Calculation of the input parameters as explained in Section 3.3.
2. Digital filtering as explained in current section.

As stated before, LSTM neural networks struggle to make accurate predictions on the prospective evolution of the filtration plant. This is mainly due to the presence of an overall trend on long term fouling conditions overlaying a set of oscillations caused by the different conditions encountered on each cycle. An oscillating behaviour over time is a much easier pattern to predict, whereas the overall trend poses a challenge to our dynamic neural network. For this reason, we have decided to split apart the training dataset. Oscillations, on one hand, will train the LSTM neural network; the general trend on the other, will train the multilayer feed forward static network.

The separation is performed by digitally filtering the training dataset. We implement a low pass FIR filter to do so. There are several parameters that affect filter design and whose values merit discussion:

- **Sample frequency**: In our case, there is no actual sample rate since values are taken once per cycle, each time our software calculates TMP_0 and R_0. This cycle does not have a constant duration.
- **Cut-off frequency**: Since our signal values are not taken at a constant rate, we cannot properly state a certain value for this parameter in Hz. Nevertheless the input parameter to the Matlab function that implements the FIR filter is the normalised cut-off frequency, which results from dividing the desired frequency by half the sample frequency (Nyquist frequency). Although the sample frequency concept has no physical meaning in our case, this relative magnitude makes perfect sense. An empirically determined suitable value for this normalised frequency would be 0.0008. Lower or higher values have yielded similar results in the final accuracy of the network. Low cut-off frequencies result in more oscillations filtered. Therefore, the obtained trend for the static prediction tends to be smooth and easy to model, whereas the oscillations that become input data for the dynamic part of the prediction are higher and harder to predict. They are usually well predicted though; the downside is that this requires a longer training period for the neural network.
- **Filter order**: Higher order filters produce a more ideal response, but involve more calculation and storage. A default Hamming window is applied to the sample collection before filtering. A number of samples equal to half of the filter order are smashed by the window's transfer function at each end of the collection. This is not an issue for the initial part of the data, but for the final one it is, since prediction will have to start before the identities of smashed samples are known, despite their actual values being established in the output.
- **Group delay**: Filtering introduces time delay in the signal. This means that the output signal is time shifted with respect to the input. This needs to be considered and solved otherwise our training dataset will not match after filtering. This is simple though: calculate group delay in terms of samples and shift the output signal back in time the same amount before joining the rest of the data for neural network training.

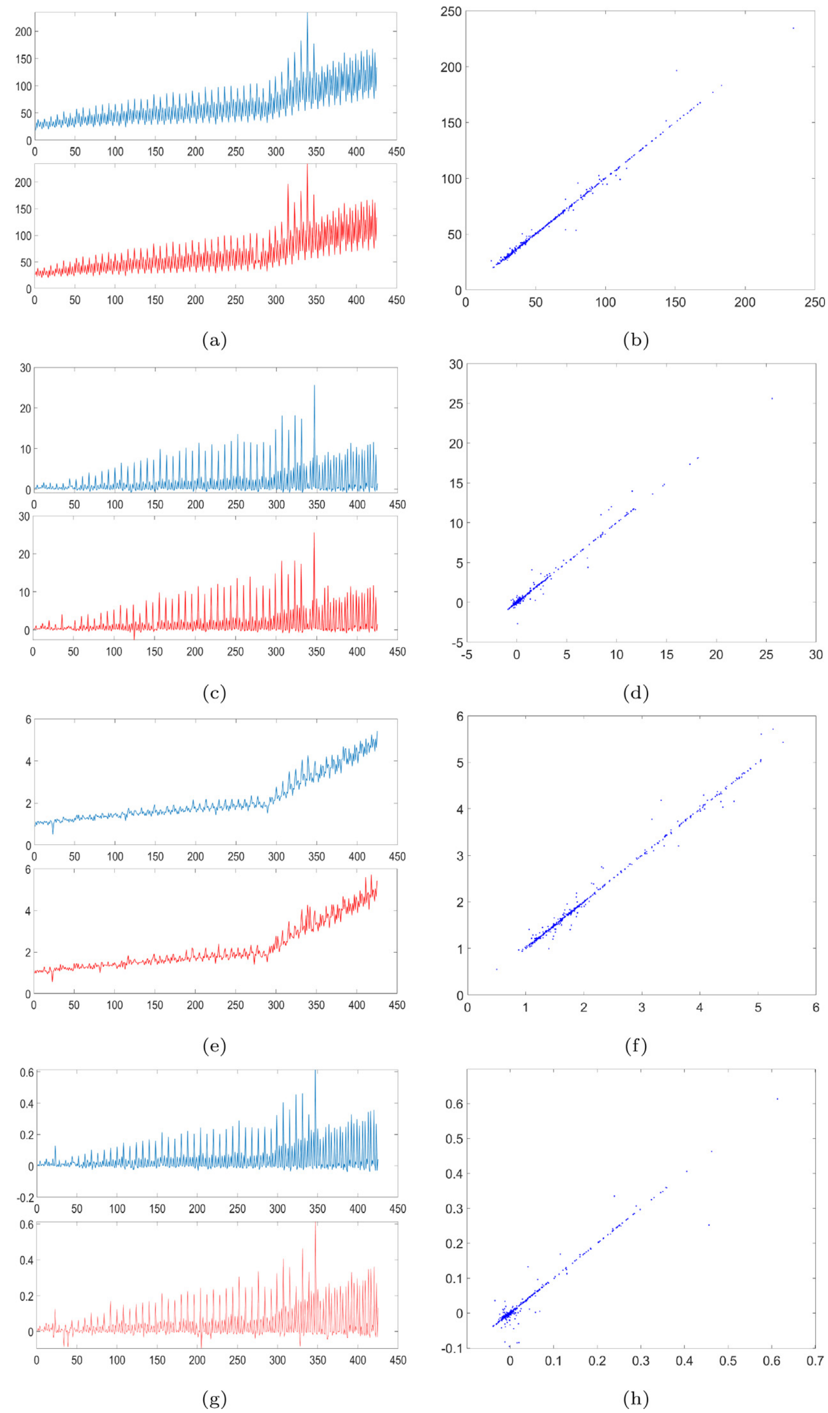


Fig. 8. Simulation results after modelling. Observed (blue) and simulated (red) values on the left, simulated vs observed values on the right: TMP_0 (mbar) (a, b). $dTMP_0/dt$ (c, d), R_0 (m^{-1}) (e, f) and dR_0/dt (g, h)

4. Results and discussion

4.1. Characterisation of membrane status (modelling)

Some previous works have been based on a dataset collected throughout a short period, so the age of the membrane could be considered constant. Other works have considered longer time spans and have required a measure of time as an approximation to the status of the membrane to achieve accurate predictions. We can assure that not doing so leads to a model that reflects short terms changes in output variables but fails to predict long term fouling.

Time has been the ageing factor and therefore the input variable in all previous works we have examined. To us it presents a problem though. Our process chains filtration and backwash periods with durations that also change over time. Sampling the process at regular intervals as it is usually done, would yield a huge set of data conforming a confusing pattern. In Mirbagheri et al. (2015a) operating conditions change significantly over time but, in our case, they reverse many times within the same experiment. Filtration and backwash cycles alternate and produce membrane fouling going up and down time and again. We thus needed to come up with a different way to represent the current state of the membrane. In Geißler et al. (2005) an hourly average is taken and seems to work well. However, we have preferred to take

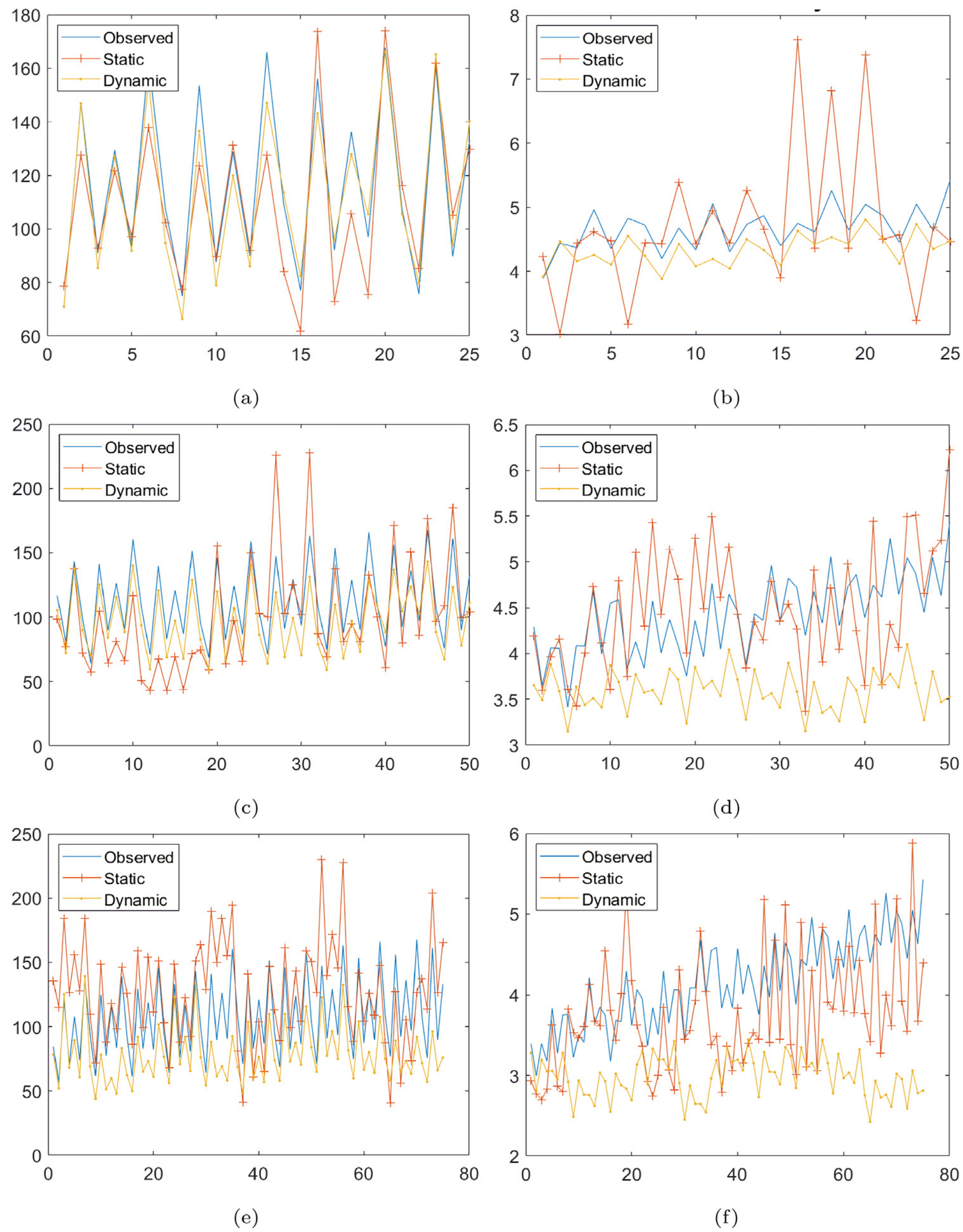


Fig. 9. 25 cycle prediction for TMP_0 (a) and R_0 (b); 50 cycle prediction for TMP_0 (c) and R_0 (d); 75 cycle prediction for TMP_0 (e) and R_0 (f).

Table 3
R2 and RSME for the hydraulic resistance at the start of the filtration period (R_0) and transmembrane pressure at the beginning of the filtration period (TMP_0) for both static and dynamic predictions.

	R_0				TMP_0			
	Static		Dynamic		Static		Dynamic	
	R^2	RMSE	R^2	RMSE	R^2	RMSE	R^2	RMSE
25 cycles	0.9910	0.016	0.1030	0.0398	0.8878	10.7449	0.7455	16.1826
50 cycles	−1,6909	0,6986	−1,5578	0,6812	0.3938	24.0764	0.3320	25.2735
75 cycles	−0,2229	0.7066	−2,4458	1,0200	−1.1661	33.0519	0.3446	24.7785

samples at the end of each filtration + backwash period. We do not use time as an input parameter; instead, we take filtration and backwash cycle duration (t_c, t_{bw}) as inputs to the network.

Two more operating conditions are taken as inputs: filtration flux (J) and backwash flux (J_{bw}).

These are the four input variables we believe are paramount to describe the behaviour of the filtration unit. Nevertheless, a measure of the status of the system is still to be defined. Time could be used but it would be a measure of the accumulated time after each filtration + backwash cycle. A second option would be the use of the accumulated volume of water already filtrated. Results were significantly better when taking volume as an input, so we decided to use volume for the rest of the work.

Fig. 8 compares the observed and simulated patterns for TMP_0, $(dTMP_0/dt)_{rev}$, R_0 and $(dR_0/dt)_{rev}$. The graphs on the right show

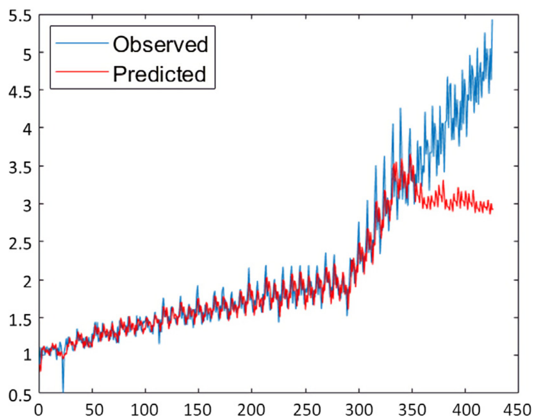


Fig. 10. Mid-term prediction on R_0 (75 cycles).

how close the model is to the original behaviour of the membranes. A straight line in the form $y = x$ would be the perfect result in this case.

4.2. Short-term prediction

In this section we compare the predictions we can make for a set of 25, 50 and 75 cycles after having trained the networks on a 400, 375 and 350-point datasets. R_0 and TMP_0 patterns are depicted in Fig. 9.

Table 3 shows a performance summary of these predictions. Training times are around 2 min for the static network and over 10 min for the dynamic one. The number of training epochs has been set to 2000 for both.

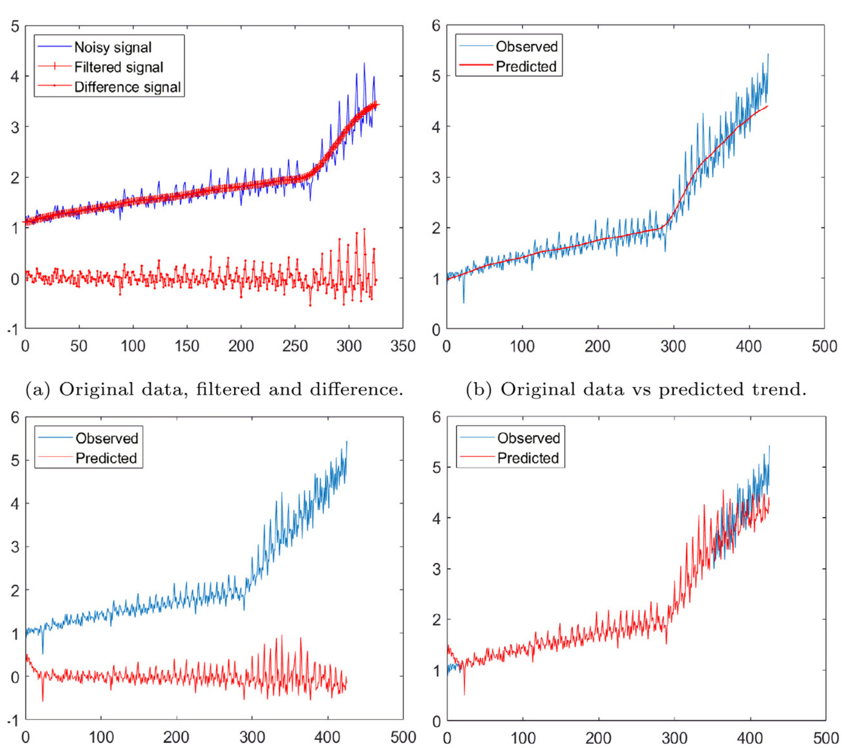
Predictions on TMP_0 are good enough up to 50 cycles ahead. The dynamic network generates more accurate responses in both cases though. 25 cycle prediction on R_0 is better when provided by a dynamic network but not so much when the output comes from the static one. However, the dynamic network makes worse predictions on R_0 for longer periods. It suggests a rule that is confirmed in the next experiments and will also lead our coming work: the dynamic network produces a prediction that corresponds quite closely in shape to the original data but separates gradually from it, whereas the static network provides a prediction increasingly different in shape but, fluctuating around the original data. Either way, predictions on the behaviour of R_0 are not reliable beyond the initial 25 cycle example. For TMP_0, this can be extended to the 50-cycle prediction example but certainly not much further than that.

Each 25-cycle chunk accounts for approximately 4 h of continuous operation. This is a good start but not our final goal. We aim to predict the network's behaviour at least a whole day of operation ahead. On our dataset, the prediction is accurate enough again for approximately 4 h but, after that, predicted output deviates from the observed one. Predicted values tend to settle after this relatively short period of time whereas the observed ones keep steadily growing. The reason for this is a widely accepted flaw on neural networks and LSTM networks in particular: they fail to adjust to trending datasets and ours shows a clear upward trend (Bandara et al., 2017).

Prediction of membrane resistance has revealed itself to be the most challenging. For the rest of the work, we will stick to this parameter, assuming that the decisions made for it will yield better results when applied to the rest of outputs.

4.3. Mid-term prediction

As seen from the previous description, anticipating responses beyond a few hours is hard. Depending on the time evolution of the dataset, some more extended predictions have been achieved but not reliably enough, since different results were obtained on the same dataset and with equal settings.



(a) Original data, filtered and difference. (b) Original data vs predicted trend.

(c) Compared original data vs fluctuations. (d) Original data vs trend + oscillations.

Fig. 11. 75 cycle prediction for R_0 using data filtration.

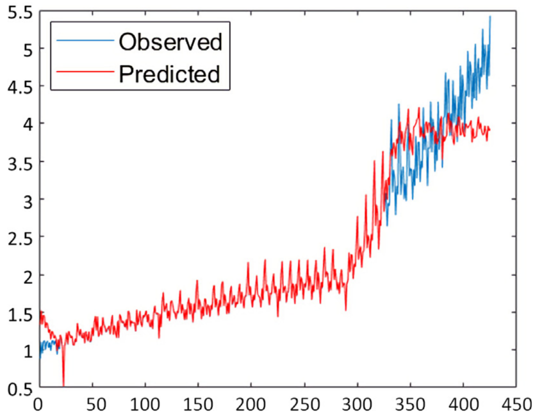


Fig. 12. Mid-term prediction on R_0 (100 cycles). Experience 1.

We have trained an LSTM network on the first 350 data from the previously mentioned 425-point dataset. The purpose is to make a prediction over the 75 remaining data and compare it with the observed data (Fig. 10). The network anticipates oscillations but fails to follow the growing trend on the evolution of R_0. We have conducted numerous tests on different datasets and network settings. Accurate predictions do not reach beyond 4–6 h ahead.

4.4. Prediction results

In this section we apply the separate prediction of general trend and oscillations over three different datasets, representing very different fouling conditions:

- Experience 1: the 425 samples pattern presented in previous sections corresponding to highly fouled membranes, particularly for the second half of the dataset.
- Experience 2: an 880 samples dataset representing a situation where membranes are clean, and the quality of the water is also good.
- Experience 3: a 455 samples dataset representing an intermediate situation.

Fig. 11 illustrates the whole process for experience 1: filtering, static prediction of the overall fouling trend, prediction of fluctuations and the final addition of the two previous predictions, compared with the actual behaviour of the membranes.

The new prediction over 75 cycles has clearly improved. Yet, it is important to note that, due to the effect of the filtering process, the first 25 of them need to be known beforehand so, the current capacity to look ahead in time is only 50 cycles. Values of R^2 and RMSE over the predicted data are 0,5589 and 0,2829 respectively. In Fig. 12 we see now what happens when trying to anticipate 25 more cycles. Predictions are not accurate this time. Taking a closer look at the pattern, it is normal though. As the training dataset is shortened at its most recent end, most of the information belongs to the initial less steep trend so the network tends to predict a more settled behaviour.

Results of experience 2 are displayed in Fig. 13.

The two previous experiences correspond to two totally different and extreme states of the membranes in the filtration tank. The first one displays a highly fouled filtration unit, whereas in the second, the membranes are clean and working under very mild conditions. A more common scenario is presented in experience 3 (Fig. 14).

This prediction is clearly accurate, making it hard to tell real and simulated data. The combined prediction works best for these types of patterns. However, we do not know beforehand how they are going to look. We then need to find a procedure to detect and correct mispredictions.

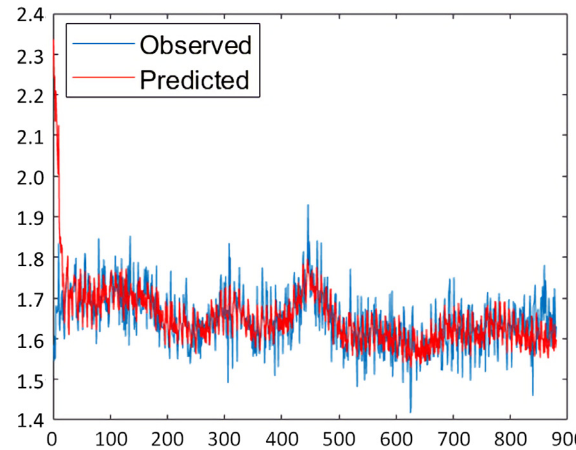


Fig. 13. Mid-term prediction on R_0 (75 cycles). Experience 2.

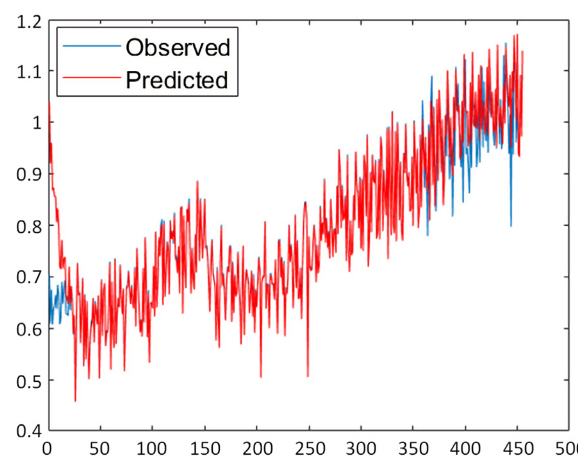


Fig. 14. Mid-term prediction on R_0 (75 cycles). Experience 3.

4.5. Retraining

An early conclusion we extract from the previous experiments is that, beyond a certain amount training data, results do not get better. We have tried 425, 455 and 880 cycle datasets and found no impact of their length on the results. Apart from the graphs already displayed, more experiments conducted, point in the same direction. Furthermore, when working conditions of the membranes change over time, old behaviour may negatively influence network training. This is what we have found in our most challenging 425-cycle dataset. There, the initial gentle slope leads to wrong predictions when not enough cycles from the second, steeper stretch of the output, are used for training.

The way this can be improved is by periodic and automated retraining of the network. Rapidly changing patterns will need more frequent retraining over relatively short datasets to avoid old patterns from influencing new predictions. Steady patterns require little or no retraining at all. A sliding window of data has been used to illustrate this procedure. This technique has already been introduced by Nam et al. (2021). The decisions to be made are how many samples the window should include and how many cycles will the network anticipate based on those samples. From the three datasets proposed so far, it makes more sense to work on the 425-cycle one, since it is the more challenging. The two decisions would make no significant effect on the remaining. Several choices of number of training samples and cycles to

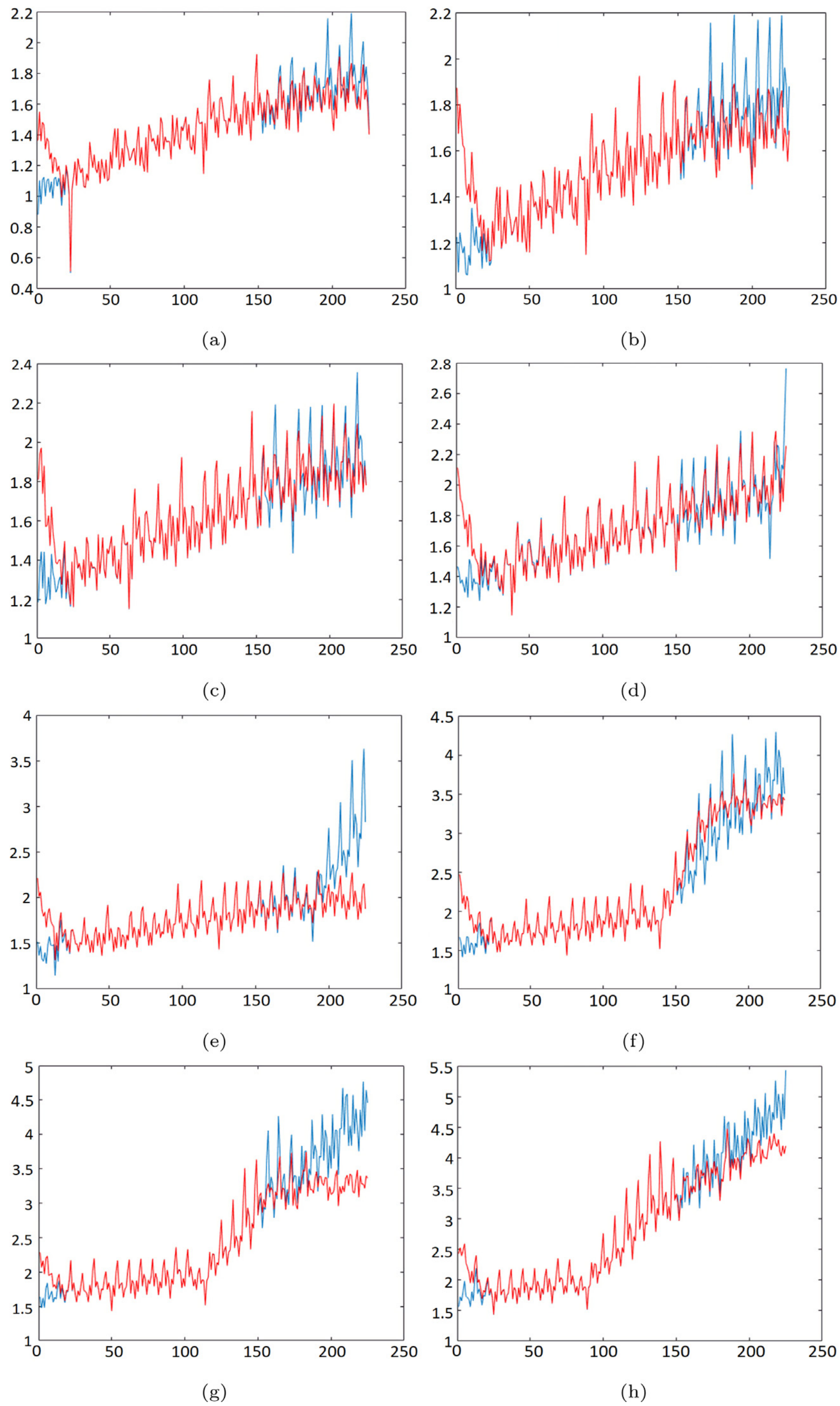


Fig. 15. Prediction over 50 cycles and retraining every 25 samples. Observed values in blue and predicted values in red.

predict were tested. Here we present one of them: 150 samples training set and 75 cycles predicted (50 actually, due to the windowing effect). Retraining is performed every 25 cycles. Fig. 15 shows the evolution of the predictions along the window.

Shorter training sets improve a network's ability to adjust to changing operating conditions but, when too short, predictions on current operating conditions may degrade. Short training sets reduce computational time, thus allowing more frequent retraining. The worst case scenario occurs when the gradient of the curve shifts right after the training dataset and before the predicted period. Predictions before and long after the "corner" are reliable, whereas those close to it are not accurate.

5. Conclusions

Feed forward and LSTM neural networks have been used for the prediction of fouling in membrane bioreactors. Data preprocessing and network retraining minimise the effects of fluctuations and the impact of mispredictions.

The LSTM neural network produces accurate predictions of the fluctuations of the data series based on cycle times and filtration flux.

The feed forward network makes accurate predictions of the general evolution of the membrane but is unable to anticipate severe changes in fouling trend.

Up to 50 filtration cycles (between 8 and 12 h) can be predicted accurately regardless of the fouling pattern and longer predictions are also reliable under stable operating conditions. The networks have been retrained every 25 filtration cycles (between 4 and 6 h) to minimise the impact of mispredictions when shifts in fouling trend occur.

The computational complexity of the whole process is low enough to allow real time operation. Preprocessing, static network training and dynamic network training have taken 1.5 s, 2 s and 1069 s respectively, whereas execution times account for less than 1 s. This real time accurate fouling prediction capability opens up a new scope for the application of neural networks to AnMBR treatment plants.

Further research needs to be done to select new input parameters related to shifts in fouling trend in order to improve and extend the prediction of membrane behaviour. The influence of the biological processes involved in membrane fouling (Nam et al., 2021) and optimisation techniques such as gene expression programming and particle swarm algorithm (Hamedi et al., 2019), should be explored to produce more accurate predictions.

CRediT authorship contribution statement

José M. Cámara: Conceptualization, Methodology, Software, Validation, Writing – original draft, Supervision. **Victorino Diez:** Methodology, Investigation, Data curation, Writing – review & editing. **Cipriano Ramos:** Investigation, Formal Analysis, Visualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

I have made the data set available online. Url is provided in the text.

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