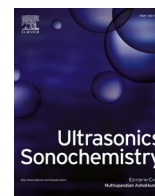


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ANN based modelling of hydrodynamic cavitation processes: Biomass pre-treatment and wastewater treatment

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ABSTRACT

We have developed artificial neural network (ANN) based models for simulating two application examples of hydrodynamic cavitation (HC) namely, biomass pre-treatment to enhance biogas and degradation of organic pollutants in water. The first case reports data on influence of number of passes through HC reactor on biogas generation from bagasse. The second case reports data on influence of HC reactor scale on degradation of dichloroaniline (DCA). Similar to most of the HC based applications, the availability of experimental data for these two applications is rather limited. In this work a systematic methodology for developing ANN model is presented. The models were shown to describe the experimental data very well. The ANN models were then evaluated for their ability to interpolate and extrapolate. Despite the limited data, the ANN models were able to simulate and interpolate the data for two very different and complex HC applications very well. The extrapolated results of biogas generation in terms of number of passes were consistent with the intuitive understanding. The extrapolated results in terms of elapsed time were however not consistent with the intuitive understanding. The ANN model was able to generate intuitively consistent extrapolated results for degradation of DCA in terms of number of passes as well as scale of HC reactor. The results will be useful for developing quantitative models of complex HC applications.

1. Introduction

Hydrodynamic cavitation (HC) is finding applications in a wide range of processes ranging from waste valorisation to specialty products. HC is a process of formation, growth and collapse of gas/vapour filled cavities in a liquid. Cavities are formed in regions where local pressure approaches the liquid's vapour pressure. These cavities grow and oscillate in a varying pressure field and subsequently collapse in a region of higher pressure. Collapse of cavities results in localised regions with intense shear and very high pressure and temperature [31,2,37]. The high pressure and temperature lead to the formation of variety of radicals including highly oxidising hydroxyl radicals. Several studies have been published outlining beneficial applications of such intense shear and hydroxyl radicals generated via hydrodynamic cavitation. For example, intense localised shear is useful to break suspended particles and finds application in disinfection [28,14,4], emulsions [22,23], pre-treatment of algae [36,35] and so on. In-situ generation of hydroxyl radicals via HC is used for treating organic pollutants in water (e.g.

[5,26,33,24]. Combination of intense shear and hydroxyl radicals have also been harnessed for a range of physico-chemical processes such as pre-treatment of waste biomass [11,18–19,3]). HC is therefore touted as a very promising platform [9,13,17].

Despite intense research and demonstrating promising potential for a wide range of applications, the potential of HC is not yet fully realised in practice mainly because of lack of computational models capable of simulating and predicting performance of HC based processes. Performance of any HC based process critically depends on number of generated cavities as well as location and intensity of their collapse. The process naturally spans over wide range of spatio-temporal scales: from a single cavity ($\sim 10 \mu\text{m}$, $\sim 10^{-4}$ s) – cluster of cavities (mm scale, $\sim 10^{-3}$ s) – cavitation reactor scale (~ 100 cm, $\sim 10^{-1}$ s). Several attempts have been made to develop quantitative understanding of cavitation processes for more than a century starting from Lord Rayleigh [25]. However, most of these single cavity models consider symmetric break-up [20]. Secondly, the cavity dynamics models require knowledge of physico-chemical properties such as thermal conductivity, diffusivity, heat capacity at extreme pressures and temperatures generated by

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Nomenclature	
<i>Acronyms:</i>	
ANN	Artificial Neural Network
BIOGAS	ANN model for describing influence of HC based pre-treatment on biomethane generation
BMP	BioMethane Potential
DCA	Di-chloro Aniline
HC	Hydrodynamic Cavitation
LCB	Ligno-cellulosic Biomass
WATER	ANN model for describing HC based degradation of DCA in water
<i>Symbols:</i>	
C	instantaneous DCA concentration
C ₀	initial DCA concentration
d	diameter of diode used for hydrodynamic cavitation
H	number of neurons in the hidden layer of ANN model
MSE	mean square error
n	number of passes for pre-treatment
N _{data}	number of experimental data points (records) available
N _{eq}	number of equations required to be solved to decide the weights for ANN model
N _{test}	number of records available to test the ANN model
N _{train}	number of records available to train the ANN model
N _{weights}	number of weights to be decided for ANN model
R	regression coefficient
R ²	coefficient of determination
t	time
X	output variable of the ANN model
<i>Subscripts:</i>	
m	model
o	observed
test	data set used for testing
train	data set for training
<i>Superscripts:</i>	
i	ith data point
–	Average over all the points in the data set

collapsed cavity. Usually, for most of the species, such information at extreme pressures (about 100 MPa) and temperatures (about 5000 K) encountered in cavity collapse is not available. In real applications, presence of other cavities and suspended particles cause significant deviations from the assumptions invoked by such cavity dynamics models. Several attempts have been made to develop multi-scale or multi-layer models combining cavity dynamics models with HC device scale models based on computational fluid dynamics (for example: [1,27,6]). However, lack of definitive understanding of micro-scale processes encountered in cavity collapse and macro-scale processes of turbulent flows with phase change still have restrained our ability to make predictive or even descriptive models of HC based processes. While efforts are being made to enhance our understanding of underlying physics and chemistry of HC, it will be useful to explore data driven approach for at least describing HC processes. Such an attempt is made here.

Chemical engineers are increasingly using artificial neural networks (ANNs) for a wide range of problems [21]. ANNs are computational tools which are capable of describing arbitrary functions. In many cases, where it is difficult to establish rigorous phenomenological models such as HC, ANNs may provide useful and practical ways of describing the complex system of interest. ANNs are based on data-driven approach which uses known inputs and outputs and an appropriate learning algorithm to establish relation between them. This enables use of ANNs for modelling, classification, prediction or optimisation [12]. ANNs' popularity has soared in recent years and they have now become one of the most sought-after artificial intelligence and machine learning tools. Artificial intelligence researchers and computer scientists are focussing on deep learning involving complex, recurrent and multi-layer architectures of ANNs. Training of such ANNs requires very large data sets relating input and output variables [34]. However, in many applications such as HC based processes: experiments are complex, time consuming and expensive which naturally imposes constraints on the amount of data which could be collected. Availability of the limited experimental data often leads to a common error of overfitting where ANN model represents the training data set so well that it captures relationships that do not exist. Such an over fitting often hinders the objective of interpolation or extrapolation which are the main goals of developing a model. In this work, we present a simple and general strategy for developing and using ANN for modelling HC based processes with limited experimental data.

Two applications studied in our group were selected for this purpose.

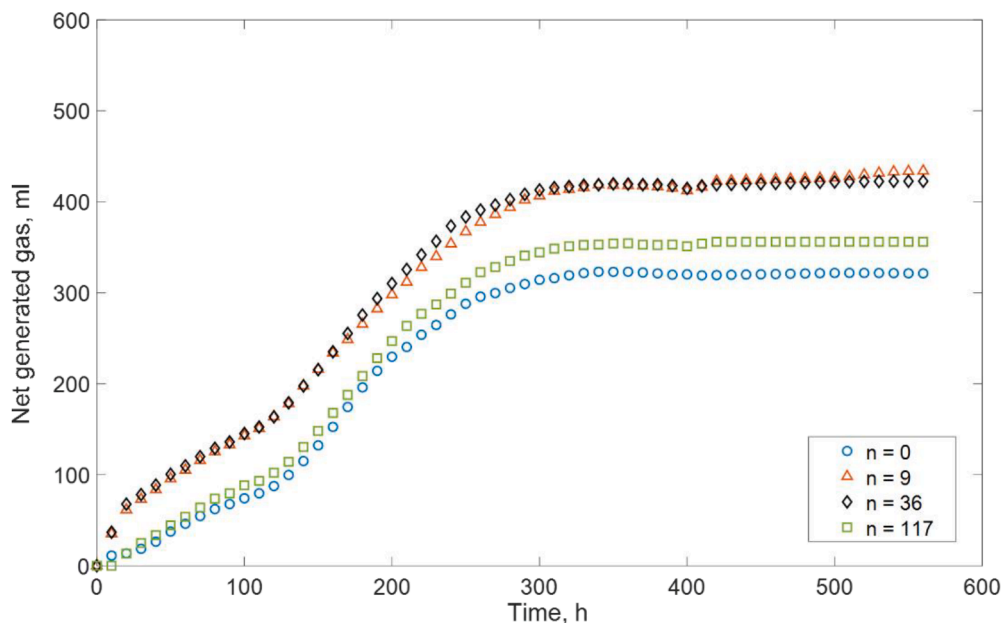
First application considered here is the use of HC for pre-treating complex biomass for enhancing biogas yield. This application and corresponding model are denoted by 'BIOGAS' in subsequent discussion. The physical effects generated via HC such as intense shear and high-speed jets modify particle size, surface area and morphology of biomass [18]. The chemical effects due to hydroxyl radicals generated via HC partially hydrolyse the carbohydrates, de-lignify LCB or reduce crystallinity [13]. These physico-chemical changes in the biomass lead to many benefits such as enhanced biogas yield. A number of reports in literature have pointed out the beneficial effects of HC pre-treatment on biogas yield [8,16,18,32,38,39]. HC seems to be the most promising pre-treatment technology for enhancing AD outputs [15]. Here we have considered a set of experiments reported by Nagarajan and Ranade [18] on the influence of HC based pre-treatment for enhancement in biogas yield (BMP) of sugar cane bagasse. The interest is in relating enhancement in BMP with the pre-treatment parameter which is number of passes through HC device. The experimental data is available only for four different number of passes, namely 0, 9, 36 and 117. Each BMP experiment takes typically one month and therefore it is impractical to carry out large number of experiments. The enhancement in BMP exhibits a maximum with respect to number of passes through the cavitation device. The desire is to use ANNs which are capable of at least interpolation and if possible, of extrapolation.

The second application considered here is wastewater treatment. The application and corresponding model are denoted by 'WATER' in subsequent discussion. HC treatment of wastewater using conventional (orifice or venturi) and contemporary (vortex based) devices have been extensively reported in literature [7,30,26,29,17]. Hydroxyl radicals generated via HC oxidise organic pollutants. The localised hot spots may also cause thermal degradation of organic pollutants to some extent and supplement radical based degradation. The degradation monotonically increases as number of passes through the cavitation device increase. However, despite several studies demonstrating effectiveness of HC for wastewater treatment, adequate information about scale-up of HC reactors is not available. There is a lack of quantitative understanding of processes occurring in HC devices and how those are affected by scale of reactor. Therefore, an ability to design and scale-up HC based wastewater treatment is severely limited. Recently, Ranade et al. [24] have for the first time reported systematic data on four geometrically similar HC reactors for degrading dichloroaniline in water (spanning volumetric flow rates over two orders of magnitude). The degradation was found to monotonically increase with number of passes through the HC reactor.

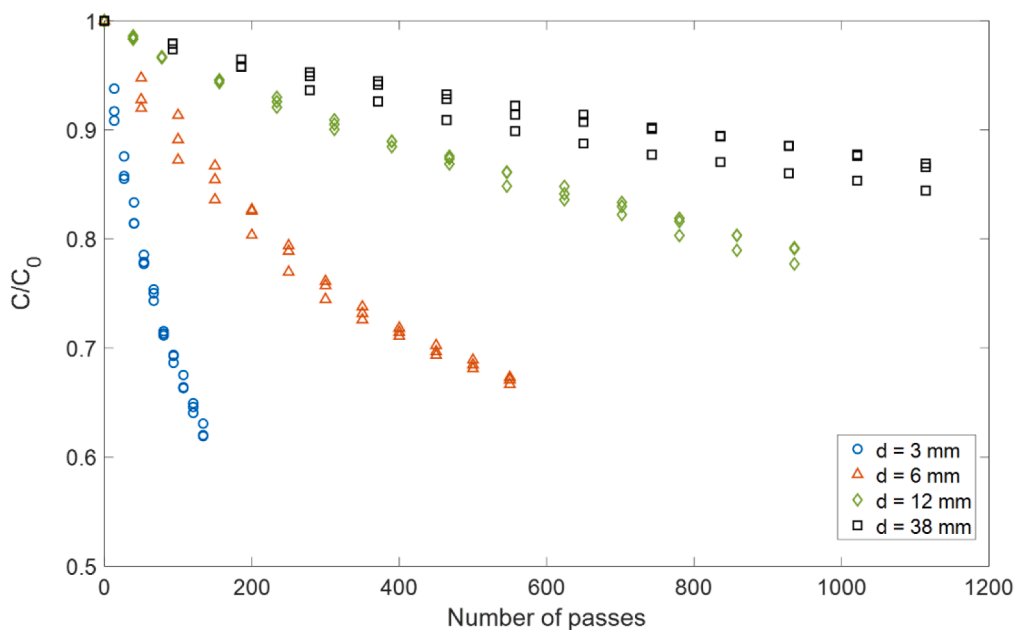
The interest is in developing a model which will allow estimation of performance of a HC reactor of any scale and thus exhibit an ability to inter as well as extrapolate.

In both these applications considered here, there are several underlying complex physical and chemical processes at work, which make it difficult to establish a phenomenological model. Hence a validated ANN model will prove very useful for these cases. The process of model development is presented in the following sections of this paper. The methods evolved are equally applicable to any discipline and hence

important. Section 2 describes the available data along with its specific characteristics to be considered while using it to train ANN. It also discusses the methods used to decide architectural details for ANN along with selection of training parameters. Section 3 presents the results. First part demonstrates and evaluates ability of ANN models to simulate reported data and provides relevant details. Hinton diagrams for weights and biases for finalised ANN models, their regression performance and simulated outputs using these models for different input conditions are reported. Ability of ANN models for interpolation and extrapolation is



(a) Influence of number of passes [n] through HC reactor on biomethane generation from bagasse (see Nagarajan and Ranade, 2019 for other details).



(b) Influence of HC reactor scale [d] on degradation of DCA with respect to number of passes [n] (see Ranade et al. 2020 for other details). C denotes DCA concentration. C₀ denotes initial concentration

Fig. 1. Experimental data used for developing ANN model.

then evaluated and discussed. Summary of the work done and key conclusions regarding the use and limitations of ANN for HC based processes are captured in Section 3. To the author's knowledge, this work for the first time, demonstrates excellent ability of ANN models to interpolate and reasonably extrapolate for such complex HC applications using rather limited experimental data. The presented approach and results will be useful for many other HC based applications.

2. Data and development of ANN model

ANN modelling is a data driven technique. ANN model for biomass pre-treatment application was developed using the data reported by Nagarajan and Ranade [18]. They report experimental data of biogas generation from bagasse with respect to time for different number of passes through HC reactor used for pre-treatment. For the wastewater treatment application, the data reported by Ranade et al. [24] was used. They report variation of concentration of pollutant (DCA) with respect to number of passes through HC reactor for four sizes of geometrically similar HC reactors. In the first part of this section, data used for developing ANN model and pre-processing of it is discussed. The subsequent two subsections discuss the methodology for selecting architecture of ANN model and training of the selected ANN model.

2.1. Data and its curation

Raw data on biomass pre-treatment and wastewater treatment used in the present work is shown in Fig. 1a and 1b respectively. Biogas generation was recorded every hour for slurry treated by 0, 9, 36 and 117 passes through the HC reactor. Please note that the data in Fig. 1a is shown at every 10 hrs for the sake of clarity though the hourly data was used for development of ANN models. Data for 566 h was available for each value of number of passes. Since the aim was to capture the dependency of biogas generation on number of passes used in pre-treatment, one input variable to the model was the number of passes. The generated biogas was recorded as a function of time. Therefore, the second input variable for the model was time. As a result, the biogas generated, which is a single output variable, was treated as a function of two input variables, time and number of passes through HC reactor. The first step in the processing of this data was to filter the data for each pass using a 24 h moving average filter. This resulted in a smoothing effect which was necessary to avoid potential problems due to overfitting. Further observation indicated that there was a slight decrease in the value of generated gas (maximum absolute magnitude of 0.1) beyond 499 h. This is physically unrealistic and therefore, the data was further curbed to 500 points each for the four passes. As a result, the data consisted of 2000 records of gas output as a function of time and number of passes. Preliminary attempts to train ANN model using the data indicated potential deviation from zero value of generated gas at time equal to zero. In order to reinforce training to ensure zero value of generated gas at time equal to zero, the data was artificially augmented by adding 500 data points of zero generated gas at time equal to zero at different number of passes. This ensured physically realistic zero generated gas at time equal to zero.

For the DCA degradation case (Fig. 1b), the data of dimensionless concentration (C/C_0) was available with respect to number of passes through HC reactors of four different throat diameter values as 3, 6, 12 and 38 mm. Experiments were repeated three times so that for a HC reactor and a particular number of passes, three values of C/C_0 were available. Data of C/C_0 corresponding to 3 mm diameter device was recorded for 11 different number of passes ranging from 0 to 134 giving 33 records. Data for 6 mm device was recorded for 12 different number of passes ranging from 0 to 550 giving 36 records. Similarly, data for 12 mm and 38 mm device was recorded for 14 and 13 different number of passes in the range 0 to 936 and 0 to 1115 respectively giving 42 and 39 additional records. Thus, total of 150 (33 + 36 + 42 + 39) records of C/C_0 , which is an output variable, were available as a function of two input

parameters, namely number of passes and diameter of HC reactor used for water treatment. Data augmentation could be done by making use of the fact that for any value of diameter when number of passes is zero, there would be no degradation of pollutant, resulting in C/C_0 value equal to 1. Fifty additional records with number of passes equal to zero and C/C_0 value equal to 1 were added for different diameter values to ensure physically realistic zero degradation at zero number of passes through HC reactor.

2.2. ANN architecture

In this work, we used MATLAB R2020a platform to construct the desired ANN models. Specifically, the 'network' function available for building custom shallow neural networks was used. Architecture of ANN is defined by number of neurons in input, output and hidden layers, along with their interconnections. This section presents the custom design of architecture for the considered two applications: BIOGAS and WATER. The corresponding ANN models are also denoted by the same names. The architecture of the ANN models comprises of input layer containing number of neurons equal to number of independent input variables, output layer containing number of neurons equal to number of outputs and single or multiple hidden layers containing neurons adequate to represent the data. Considering that both the applications, BIOGAS and WATER have two independent input variables and one output variable, the ANN architecture of both the models had two neurons in the input layer and one neuron in the output layer. Parameters of the developed ANN model are summarised in Table 1.

One hidden layer was chosen as it is reported that a single hidden layer can approximate any function that contains a continuous mapping from one finite space to another [10]. The maximum number of neurons in hidden layer could be decided by considering the number of weights to be decided in the process of training the network. The number of weights (N_{weight}) are related to number of neurons (H) in the hidden layer for input size 2 and output size 1 by Equation (1):

$$N_{weight} = 2 \times H + 1 \times H \quad (1)$$

Number of records available for training (N_{train}) decide the number of equations (N_{eq}) used to solve while finding the weights. N_{train} should be at least some multiples of number of weights to be decided (N_{weight}). Otherwise it causes overfitting; which means better fitting to training data but less generalisation for unseen data. A general thumb rule is to take N_{train} as at least ten times of N_{weight} . Considering this thumb rule, Equation (1) and assuming that 70% of the available data is used for training, the number of neurons, H , in the single hidden layer used for the BIOGAS and WATER ANN models may be written as:

$$H \leq \frac{0.7 \times N_{data}}{3 \times 10} \quad (2)$$

N_{data} is number of experimental data points available. Using Equation (2) the maximum number of neurons in hidden layer for the BIOGAS model would be about 60 since total data points available are 2500. For the WATER model, the available data points are 200 and therefore

Table 1
Key parameters of the selected ANN models.

Network Property	BIOGAS model	WATER model
Input layer size	2	2
Output layer size	1	1
Hidden layer size	10	4
Hidden layer transfer function	'tansig'	'tansig'
Output layer transfer function	'purelin'	'purelin'
Data pre/ post processing	'mapminmax' [0 1]	'mapminmax' [0 1]
Training function	'trainlm'	'trainlm'
Performance function	'mse'	'mse'
Data division (ratio)	'dividerand' (70:15:15)	'dividerand' (70:15:15)
Train parameter goal	0.01	0.0

maximum number of neurons would be about 5.

Using this general guidance, several network models with variable number of neurons were created and tested for their performance. For the BIOGAS model, number of neurons were varied from 3 to 22 and for the WATER model, number of neurons were varied from 3 to 12. Appropriate balance between fit and generalisation was achieved by evaluating coefficient of determination, R^2 (Equation (3)) and mean square error, MSE (Equation (4)) of test data.

$$R^2 = 1 - \frac{\sum_{i=1}^{N_{train}} (X_m^i - X_o^i)^2}{\sum_{i=1}^{N_{train}} (X_o^i - \bar{X}_o)^2} \quad (3)$$

$$MSE = \frac{\sum_{i=1}^{N_{test}} (X_m^i - X_o^i)^2}{N_{test}} \quad (4)$$

Where X is a modelled variable, superscript i denotes i^{th} record and subscripts m and o denote modelled and observed data respectively. N_{train} is number of records used for training and N_{test} is number of records used for testing. It follows from Equation (3) that the value of R^2 becomes one when modelled values exactly match observed values. Appropriate number of neurons in the hidden layer were hence selected by ensuring the coefficient of determination (R^2) is higher than 0.99 and error in estimating the test data is minimum. Results and more details are discussed in Section 3.1.

2.3. ANN training

Training a neural network is the process of finding weights and biases so that computed outputs are close to the observed values or targets for a collection of training records. 'train' function of MATLAB was used in this work for training the developed shallow network models. It implements batch training such that during one epoch of training all input vectors are presented to the network and then the weights are updated. Initially, two different functions 'trainlm' and 'trainbr' were evaluated for training. Both the functions have back propagation algorithm which uses the Levenberg-Marquardt optimization. The 'trainbr' additionally uses Bayesian regularization. The results of 'trainlm' were found to be superior than the 'trainbr' and was therefore selected for further work. The available data was divided into three sets as training, validation and testing. The terminologies of 'train', 'validate' and 'test' used here refer to MATLAB terminology to partition the available data. 70% of the available data was used for training and the remaining 30% was divided equally for validation and testing. This was done by adjusting the 'divideParam'. This data division as 70:15:15 for train, validate and test was used in both the models, BIOGAS and WATER. The inputs to both models were normalised by setting 'processFcn' for each input to 'mapminmax' with a range [0 1].

For different number of hidden layer neurons, hundred networks were trained for each case. These hundred models differed in their initial weights and the random division of data set. Thus, 2000 (20 different values of neurons X 100) models were created for the BIOGAS application and 1000 (10 different values of neurons X 100) models were created for the WATER application. Their performance was recorded as the R^2 . The real test for any ANN model is the way it responds to unseen data. Therefore, performance for only test data was also recorded for each model as value of 'tr.best_tperf' which gives mean square error (MSE) in fitting the test data. Key parameters of final networks selected for considered cases are listed in Table 1. The results obtained using these ANN models are discussed in the following section.

3. Results and discussion

The results used for selecting ANN architecture are discussed first. The comparison of simulated results and the experimental data is presented in Section 3.2. Besides comparing the simulated results with the

experimental data, the performance of the finalised ANN models was also evaluated by examining an ability of the ANN models to interpolate the results within the considered parameter range. Possibility of using the ANN models for extrapolation is evaluated and discussed in Section 3.3.

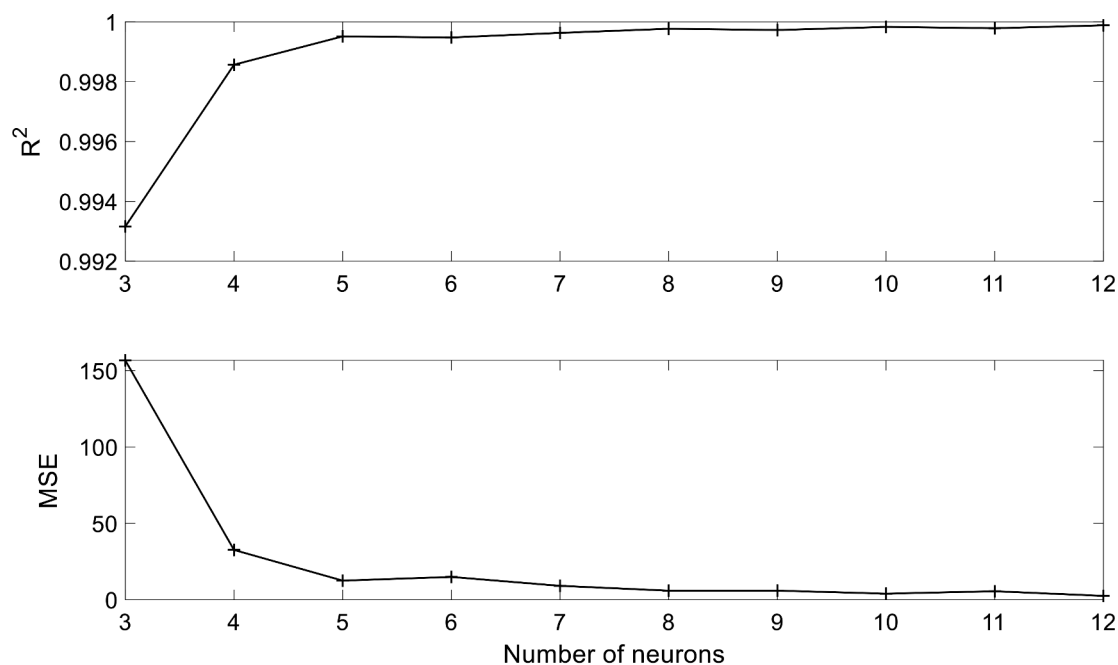
3.1. Finalising ANN models for BIOGAS and WATER applications

As mentioned in Section 2, the final ANN models were selected by comparing performance of hundred networks for each value of neurons in hidden layer. Each network differs in its starting weights, biases and the division of training records. As a result, it converges to different state after its training is complete. The performance of these networks is therefore different for a given data. Maximum value of R^2 and minimum value of MSE for unseen test data as a function of number of neurons in the hidden layer for BIOGAS and WATER models are shown in Fig. 2a and 2b respectively. It can be seen that for BIOGAS model, R^2 increases and MSE decreases with increase in the number of neurons from 3 to 22. The results up to 12 neurons are shown in Fig. 2a. The results for neurons from 13 to 22 are shown in Figure S1 of the supplementary information. R^2 is above 0.999 for 10 neurons. It was seen (Figure S1) that further increase in number of neurons from 10 to 22 resulted in only about 1% reduction in MSE than that was observed when neurons were increased from 3 to 10. It was also observed for higher number of neurons, (Figure S2) that even if R^2 was nearly equal to 1 indicating a perfect fit, the plot of generated bio-methane as function of number of passes showed a negative gas generation which is physically unrealistic. Based on these results, ten neurons were chosen for the hidden layer of BIOGAS model. The ANN with the least corresponding MSE out of 100 examined networks was selected as the final BIOGAS model for further evaluation. For the WATER model, it was observed that R^2 increased with increase in number of neurons. The MSE, however, showed a minimum at 4 neurons; MSE increased beyond that indicating an over-fit. Hence four neurons were finalised for the hidden layer of the WATER model. The ANN with the least corresponding MSE out of 100 examined networks was selected as the final WATER model for further evaluation. The 'Hinton diagrams' showing network architecture, input weights, layer weights and biases for the BIOGAS and WATER models are shown in Fig. 3a and 3b respectively. Usual MATLAB convention is followed for preparing these Hinton diagrams. The numerical values of weights and schematics of neural networks used in BIOGAS and WATER models are also embedded in Fig. 3a and 3b.

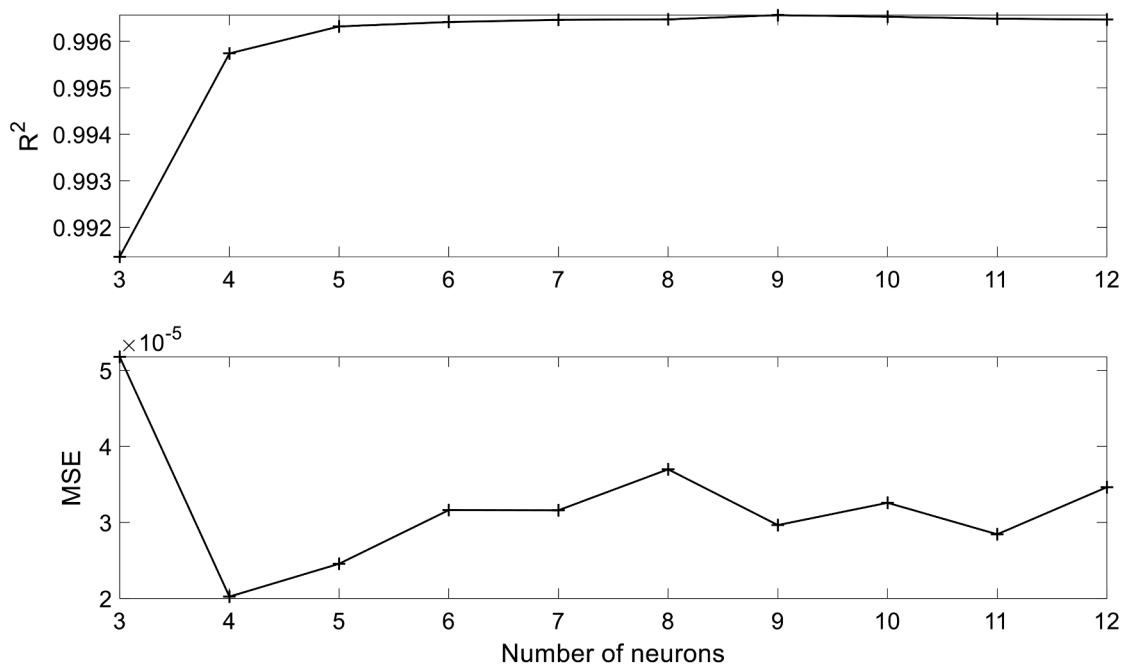
3.2. Performance of BIOGAS and WATER models

Performance of the models was evaluated in two ways. Regression coefficients for predicted values of entire data as well as only test data were calculated. The regression on entire data indicates overall quality of fit and that for only test data indicates how the model responds to unknown inputs. The comparison of results simulated for BIOGAS and WATER applications with the respective data sets is shown in Fig. 4a and 4b respectively. It is observed that BIOGAS model which had sufficient number of training records gives better values of regression coefficient for both data sets than WATER model which had relatively limited records. However, it can be seen that all four plots have a regression coefficient greater than 0.99 which is in accordance with the requirement stated in Section 2. Regression coefficients greater than 0.999 for both test data sets indicate that both the models have a very good generalization property. It also confirms that both the ANN models are able to describe the available experimental data very well.

After establishing excellent performance of the developed ANN models for describing experimental data, interpolation ability of these ANN models was investigated. Simulations were therefore carried out to predict the output variables corresponding to unknown input conditions within the experimentally studied range for both the models. The



(a) Influence of number of neurons on R^2 and MSE for BIOGAS model

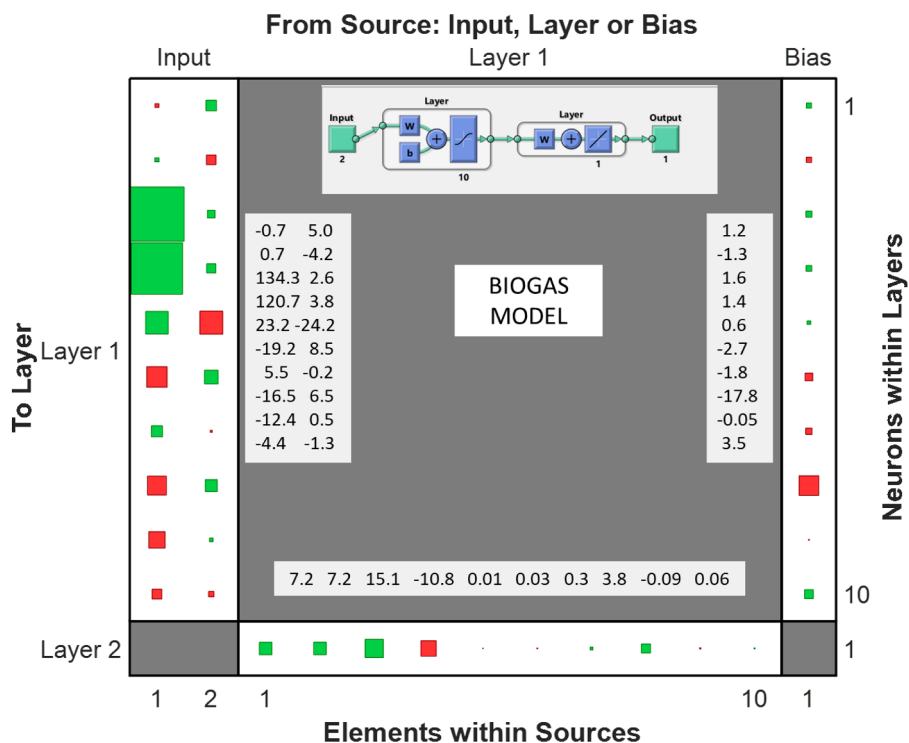


(b) Influence of number of neurons on R^2 and MSE for WATER model

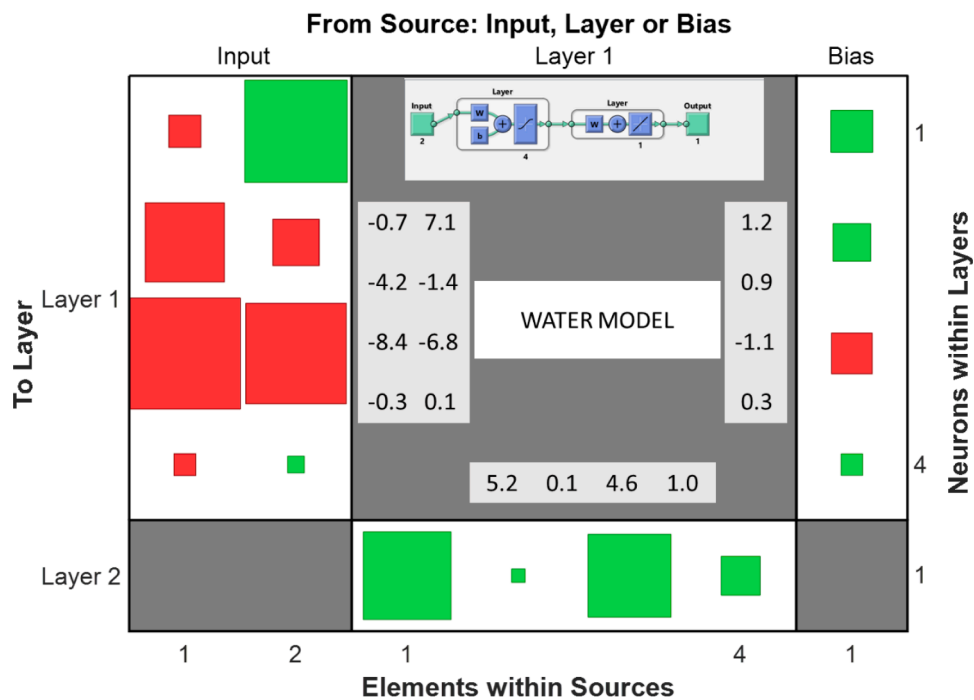
Fig. 2. Selection of number of neurons in the hidden layer of ANN models.

BIOGAS model was developed to capture the dependence of generated bio-methane on elapsed time and the number of passes used in pre-treatment of biomass. Since data for number of passes equal to 0, 9, 36 and 117 was used while developing the model, it was decided to evaluate performance of the BIOGAS model by simulating the bio-methane generation for number of passes as 5, 25, 50 and 70. Fig. 5a shows the result of these simulations. It is observed that the overall nature for all these four new cases maintains the same trend observed experimentally for number of passes equal to 0, 9, 36 and 117; that is a

rapid initial increase in gas produced followed by plateauing of it after around 300 h. It can also be observed that the case of number of passes equal to 25 shows maximum bio-methane generation within these four new cases. In order to understand influence of number of passes, the BIOGAS model was used to simulate bio-methane generation as a function of number of passes within the range from 0 to 117 with an increment of one at four different time instants ($t = 50, 100, 200$ and 400 h). These results are shown in Fig. 5b. The experimentally observed values are also marked by symbols at 0, 9, 36 and 117 number of passes.

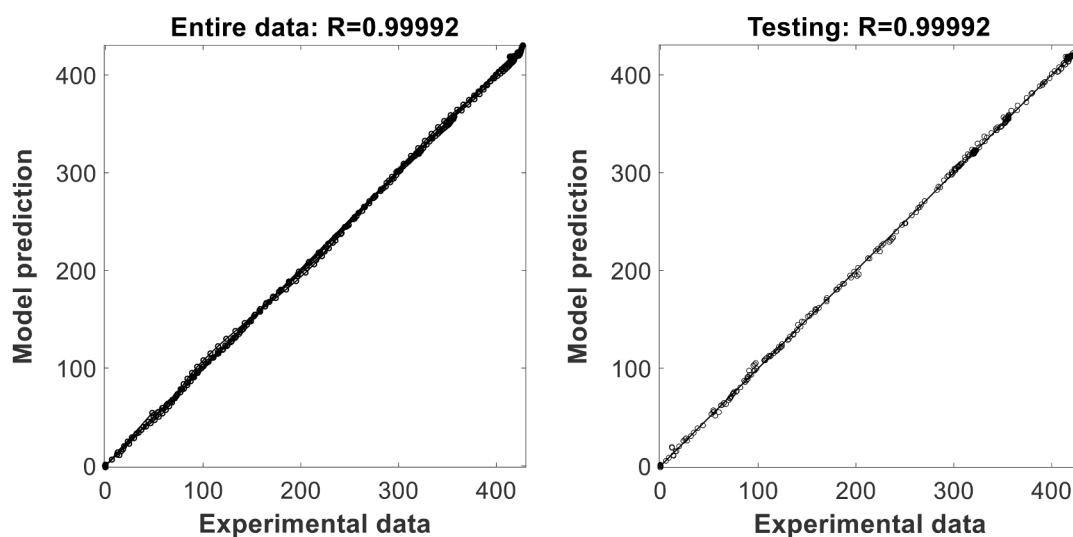


(a) Hinton diagram for BIOGAS model

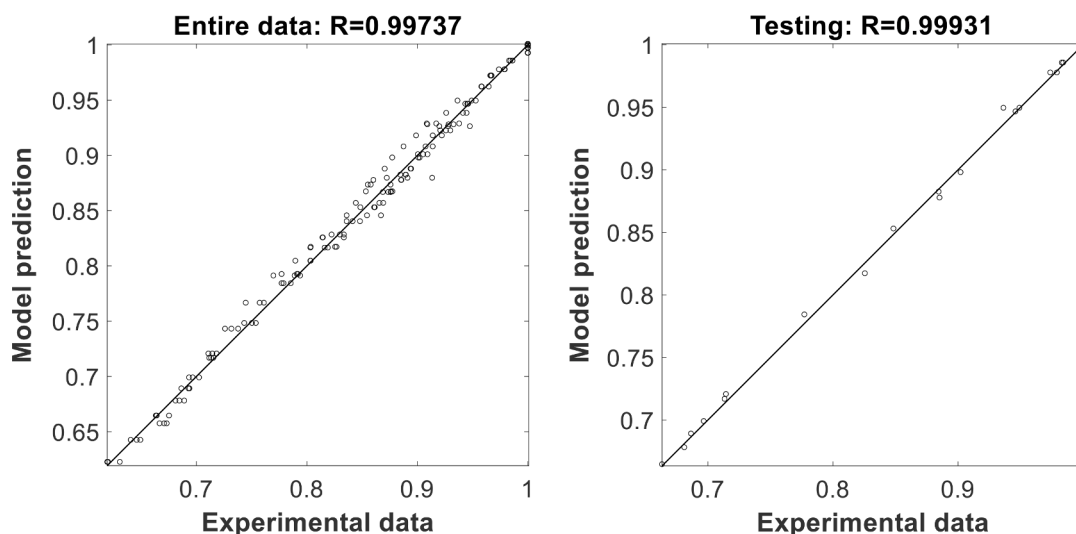


(b) Hinton diagram for WATER model

Fig. 3. Architecture, weights and biases for BIOGAS and WATER models MATLAB convention is followed: red indicates negative, green indicates positive; area is proportional to the magnitude of weights/ biases; top horizontal edge indicates source and left vertical edge indicates destination of connection; numerical values of weights are listed in grey boxes. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



(a) Parity plots for the entire and testing data sets for BIOGAS application



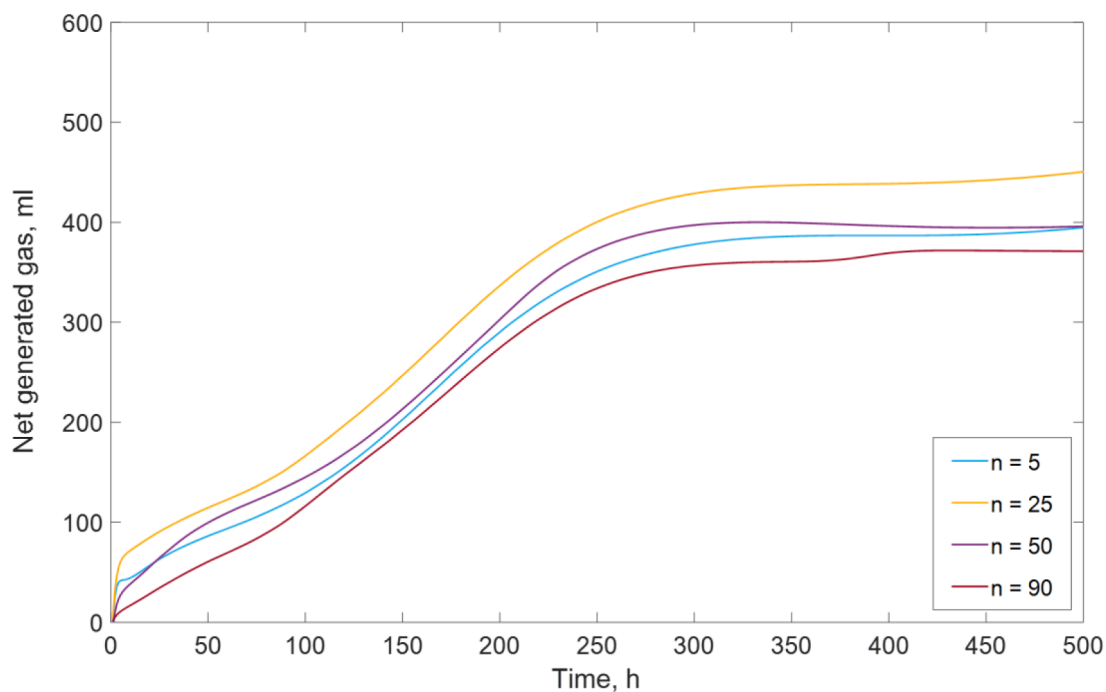
(b) Parity plots for the entire and testing data sets for WATER application

Fig. 4. Comparison of simulated and experimental data for the entire and testing data sets.

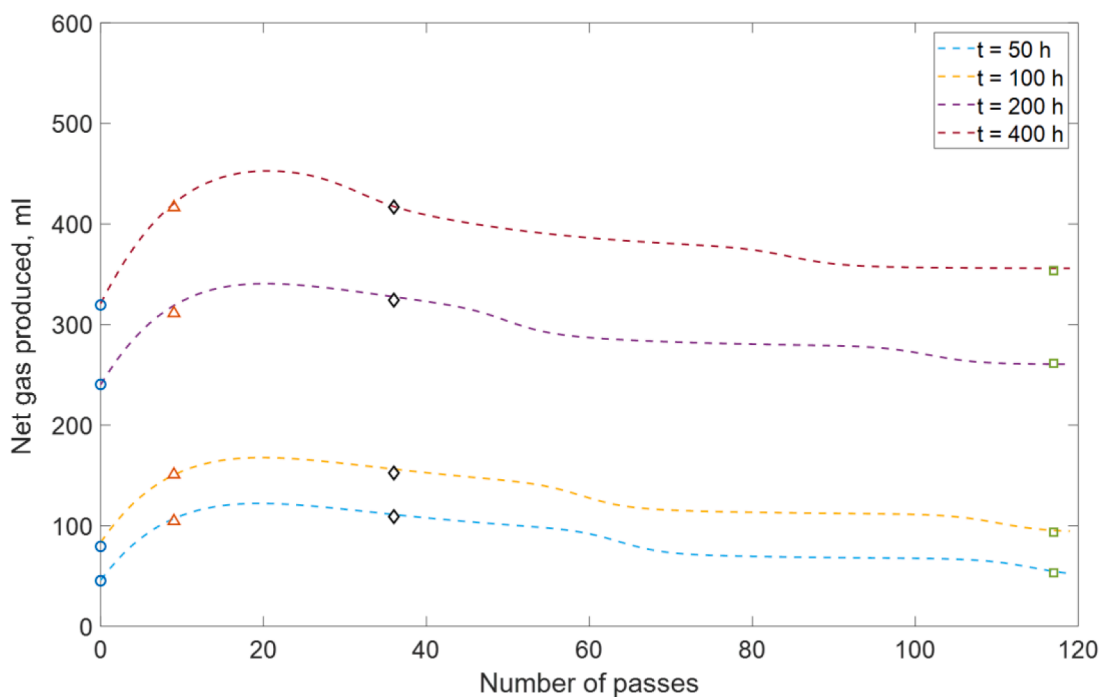
It is seen that the nature of plots at different time instants is similar. All of them show a maximum at number of passes equal to 20. The simulated results shown in Fig. 5a and 5b are consistent with intuitive understanding and the experimental data available at number of passes equal to 0, 9, 36 and 117. It can therefore be concluded that BIOGAS model not only has captured the available experimental data but also has capability to interpolate the results within the range of parameters considered for training the ANN model.

WATER model was developed to capture influence of the scale of and number of passes through the HC reactor on DCA degradation. Since experimental data for characteristic HC reactor diameter equal to 3, 6, 12 and 38 mm was used while developing the model, it was decided to simulate degradation profiles of DCA with characteristic diameter of HC reactor as 4, 10, 15 and 25 mm for evaluating the interpolation ability of the WATER model. The results of these simulations are shown in Fig. 6a. It can be seen from the simulated profiles of dimensionless concentration

of DCA that the simulated profiles follow the overall trends observed in the experimental data obtained for HC reactor diameter of 3, 6, 12, and 38 mm. All the profiles start from the dimensionless concentration of 1 and decrease with increasing number of passes. In order to further evaluate an ability of the WATER Model to interpolate with respect of HC reactor scale, simulated results of dimensionless concentration are plotted as a function of characteristic diameter of HC reactor at four different values of number of passes (50, 100, 500 and 1000). These results are shown in Fig. 6b. The experimentally observed values are also marked at HC reactor diameters as 3, 6, 12 and 38 mm in this figure. It can be seen that the simulated results shown in Fig. 6a and 6b are consistent with intuitive understanding and the experimental data available at HC reactors of characteristic diameter as 3, 6, 12 and 38 mm. It can therefore be concluded that the WATER Model not only has captured the available experimental data but also has capability to interpolate the results within the range of parameters considered for



(a) Bio-methane generation as a function of time at four number of passes



(b) Influence of number of passes at four different time instants

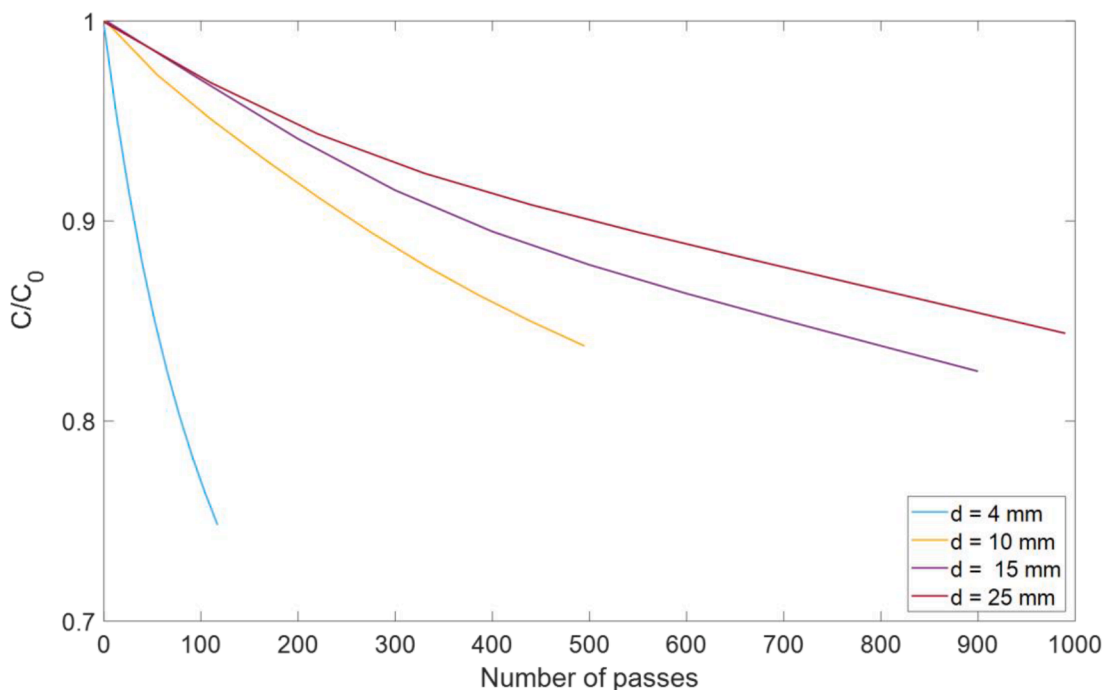
Fig. 5. Application of BIOGAS model for interpolation of results within the considered parameter range (Biomass pre-treatment for enhancing biogas).

training the ANN model.

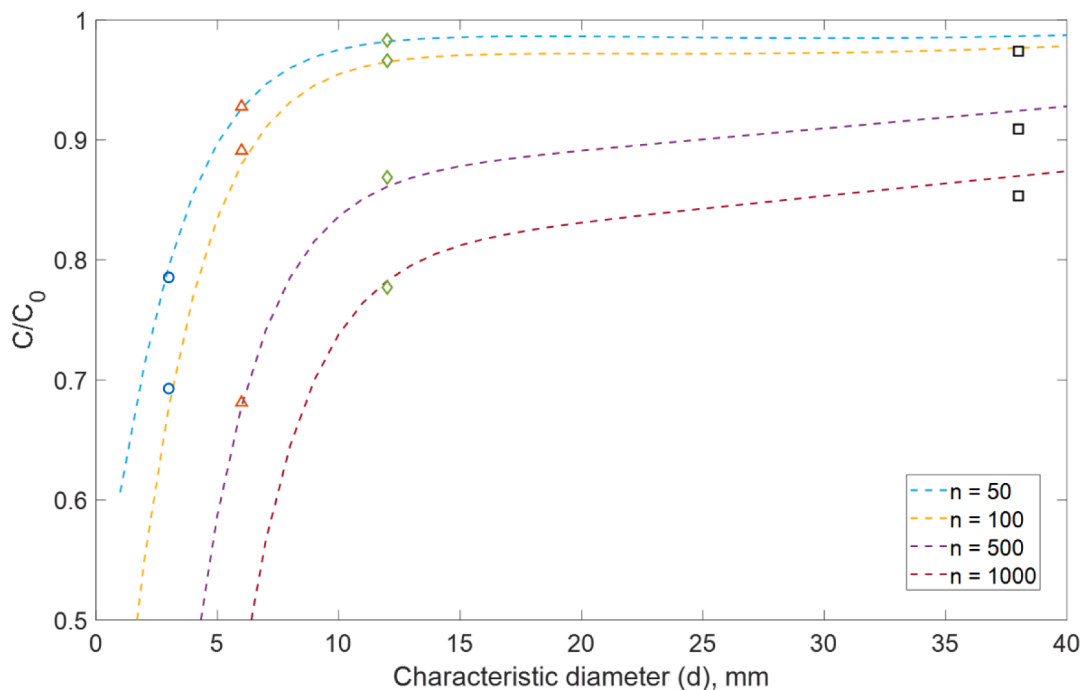
3.3. Extrapolation beyond considered parameter range

After demonstrating that the BIOGAS and WATER models were able to describe available experimental data accurately and were able to interpolate the results within the considered parameter range, it was

worthwhile to examine the performance of these ANN models for extrapolation. Considering that both the models involved two input variables, it was useful to examine extrapolation with respect to both these parameters. Qualitatively, both the models could be extrapolated in two ways:



(a) Degradation of DCA as a function of number of passes at four characteristic HC reactors



(b) Influence of characteristic diameter of HC reactor at four values of number of passes

Fig. 6. Application of WATER model for interpolation of results within the considered parameter range (Degradation of DCA in water).

- i. Extending the length of the experiments: Extrapolation in terms of time for biomass pre-treatment experiments and extrapolation in terms of number of passes for water treatment experiments.
- ii. Extending the key performance or design parameter: extrapolation in terms of number of passes for biomass pre-treatment and

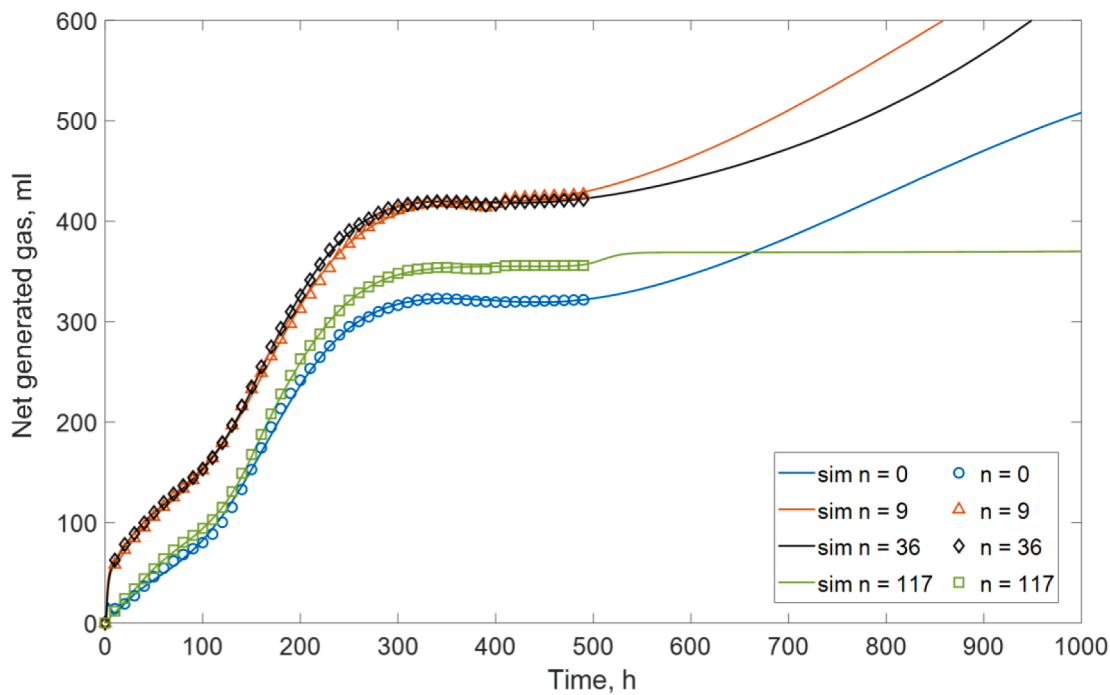
extrapolation in terms of characteristic diameter of HC reactor for water treatment.

The BIOGAS model was used to simulate bio-methane generation beyond 500 hrs and the WATER model was used to simulate degradation

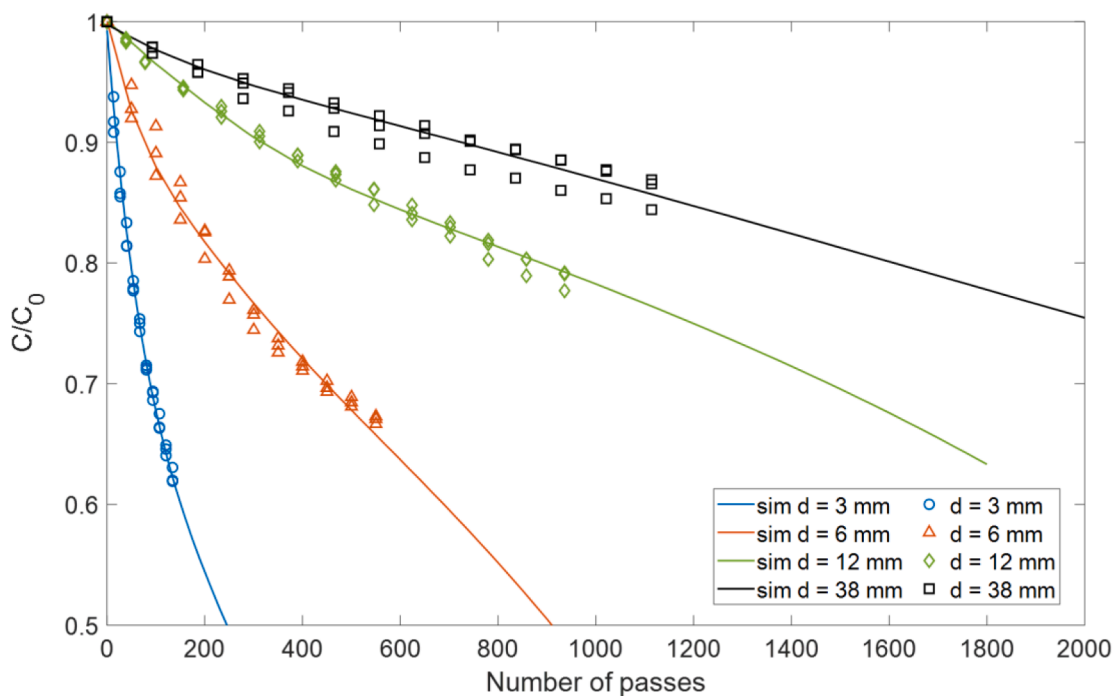
of DCA with respect to number of passes beyond those considered in the degradation of DCA experiments. These results are shown in Fig. 7a and 7b for the BIOGAS and WATER models respectively.

It can be seen from Fig. 7a that simulated results with the BIOGAS model show excellent agreement with the experimental data which is expected from the parity plots discussed earlier. However, the extrapolated bio-methane generation with respect to time shows unphysical

trends except at number of passes equal to 117. Once the bio-methane generation is plateaued with respect to time, further increase in elapsed time should not increase bio-methane generation since digestible biomass would be fully consumed by then. The BIOGAS model was able to capture this intuitively correct trend for $n = 117$. However, the simulated trends for other number of passes were not consistent with this intuitive understanding. Further work is needed to understand



(a) Simulated bio-methane generation at four different number of passes (BIOGAS model)



(b) Simulated DCA degradation profiles at four scales of HC reactor (WATER model)

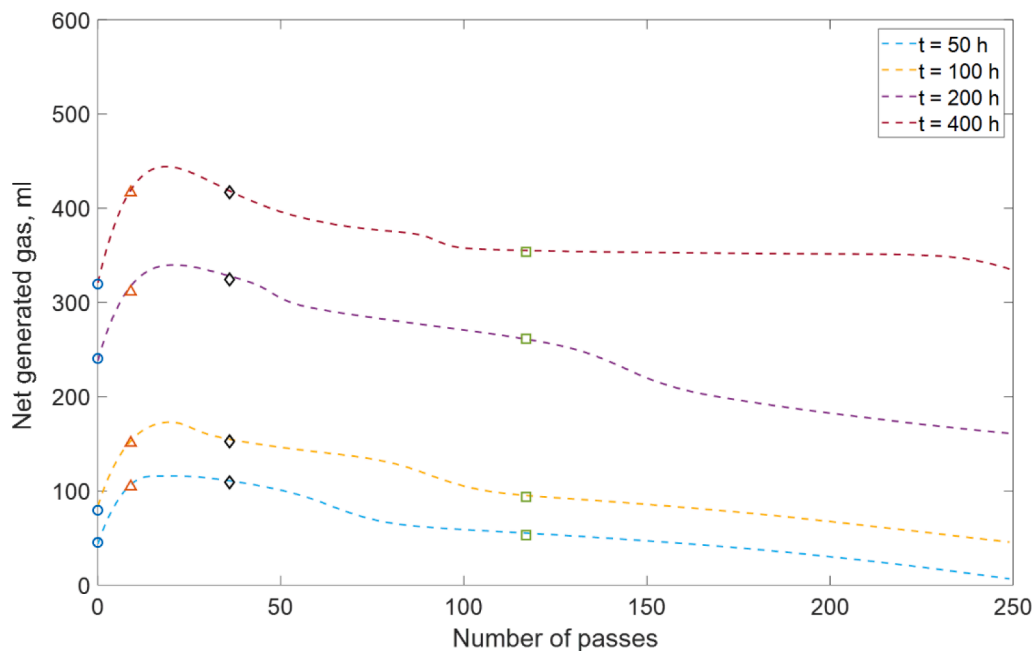
Fig. 7. Extrapolation ability of BIOGAS and WATER models with respect to time and number of passes respectively.

possible reasons for this lack of ability to extrapolate with respect to elapsed time. Unlike this, it can be seen from Fig. 7b that the WATER model was able to capture trends of DCA degradation with respect to time which are consistent with the intuitive understanding. The results not only show excellent agreement with the experimental data but also show reasonably good ability of the WATER model for extrapolation at least till the range considered in this work.

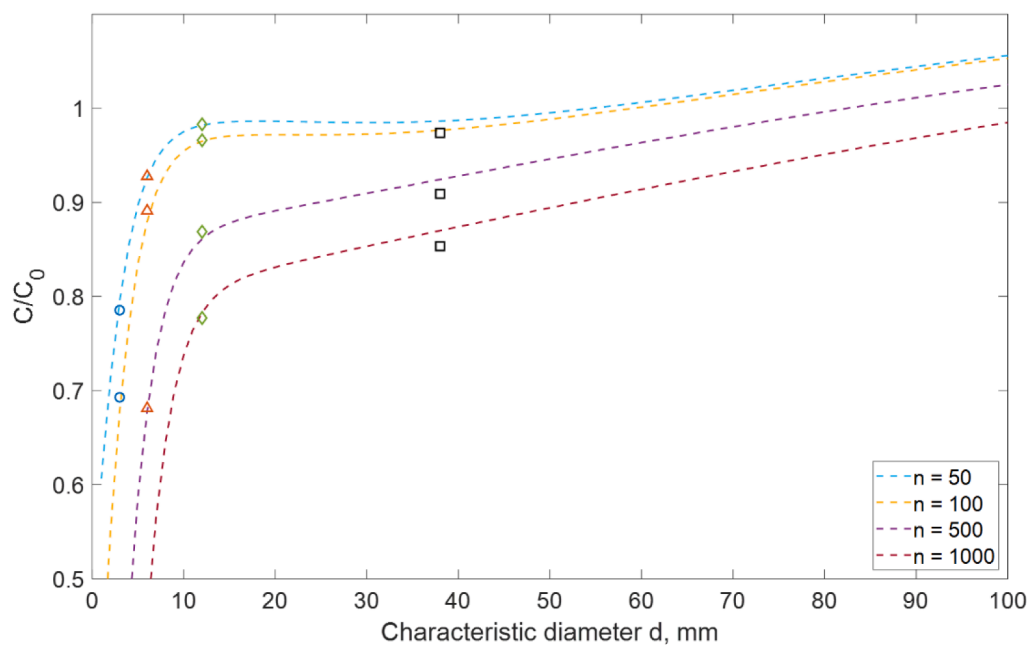
It will be very useful to examine extrapolation ability with respect to key design parameters. The BIOGAS model was therefore used to simulate influence of number of passes beyond 117. The results are

shown in Fig. 8a. It can be seen that for all four values of time instants, the BIOGAS model predicted some decrease in bio-methane generation with further increase in number of passes beyond 117. These results are consistent with the experimentally observed trends and intuitive understanding of influence of excess cavitation on bio-methane potential [18].

Considering an interest in scale-up of HC reactors for wastewater treatment, the WATER model was used to simulate influence of HC reactor scale beyond 38 mm. The predicted results are shown in Fig. 8b. It can be seen that the ANN model was able to predict results which were



(a) Predicted influence of number of passes beyond 117



(b) Predicted influence of characteristic diameter of HC reactor beyond 38 mm

Fig. 8. Extrapolation ability of Model 1 and Model 2 with respect to key design parameters.

consistent with the experimentally observed trends and intuitive understanding [24]. The results shown in Fig. 8b are also consistent with the results shown in Fig. 7b which clearly shows that the influence of HC reactor scale reduces as the scale increases and eventually points to an asymptotic nature. The asymptotic behaviour exhibited by larger scale HC reactors as discussed by Ranade et al. [24] was consistently captured by the WATER model.

The results for extrapolation were rather unexpected since in general data driven models are not expected to perform well beyond the range considered for their training. It was however heartening to see encouraging results of the ANN models developed in this work which not only were successful in describing available experimental data but were also able to show excellent interpolation ability and reasonable extrapolation ability. In absence of systematic and quantitative understanding of physics and chemistry of HC, the ANN models offer an attractive platform to model HC based processes and complex applications. As we develop better understanding and quantitative models for simulating underlying physics and chemistry, one may aim to develop better physics informed ANN models to further improve ability to extrapolate. We hope that this work stimulates further research in this promising area and will hopefully facilitate realisation of hitherto unattainable potential of HC.

4. Conclusions

ANN models were developed in this work for two illustrative applications of HC namely, biomass pre-treatment for enhancing biogas and wastewater treatment. MATLAB was used for this purpose. These ANN models were developed using a rather limited experimental data which is typical for many HC applications. A simple and general strategy for developing ANN models with a systematic methodology for selecting number of neurons in the hidden layer and selecting appropriate ANN for selected number of neurons is presented. Key conclusions of this work are:

- Appropriate number of neurons in the hidden layer and specific ANN can be selected based on coefficient of determination, R^2 (greater than 0.99) and minimising mean square error, MSE without resulting in intuitively inconsistent results. This methodology showed that 10 neurons were adequate for capturing bagasse pre-treatment data and 4 neurons were adequate for capturing DCA degradation data considered in this work.
- The ANN models were able to describe the available experimental data quite well with regression coefficient greater than 0.997.
- The developed ANN models were able to interpolate experimental data on biomass pre-treatment as well as wastewater treatment in a consistent manner.
- Extrapolation of bio-methane generation with respect to elapsed time using the developed ANN model resulted in unphysical and intuitively inconsistent results. However, ANN models were able to extrapolate bio-methane generation with respect to number of passes through HC reactor in an intuitively consistent way.
- ANN model was able to extrapolate degradation of DCA data both in terms of number of passes (elapsed time) as well as scale of HC reactor

The approach and ANN models presented in this work will be useful for simulating complex HC processes and applications in absence of quantitative phenomenological models.

CRedit authorship contribution statement

Nanda V. Ranade: Investigation, Data curation, Validation. **Sanjay Nagarajan:** Investigation, Validation. **Varaha Sarvothaman:** Investigation, Validation. **Vivek V. Ranade:** Conceptualization, Funding acquisition, Supervision.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ultsonch.2020.105428>.

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