
Applying an ANFIS-based Algorithm in Comparison with Mechanistic Modelling in a Biofilter Treating Hexane

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Abstract

Predicting the dynamic performance of a waste air biofilter is sought here. This predicting method in biological purification of waste air is adopted where the microbial biofilm formed on bed particles degrade the pollutants. The model can be adopted in scaling-up and predicting the biofiltration performance. An Adaptive Neuro-Fuzzy Inference System (ANFIS) is applied as a new approach which is compared to a mechanistic model where moisture content balance is of concern. To get a better view of each modelling procedures, they are compared for the prediction of a set of experimental data from the literature. Both of methods could effectively predict outlet concentrations.

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The results indicate a more precise predicting capability in ANFIS-based approach regarding outlet concentrations, while, mechanistic modelling has the ability of system description and mechanisms.

Keywords: Dynamic Modelling, Hexane Biofiltration, ANFIS, Gravitational Search algorithm, Moisture Content.

1 Introduction

Among the various contaminated air treatment methods, biological treatment not only requires lower investment and operating costs but it is an environment friendly technique [1]. Biofiltration is an approach for Biological purification of waste air where contaminated air is passed through a packed bed and microbial biofilm is formed on the bed particles that degrades the transferred pollutants absorbed from the air, Figure 1.

An important factor affecting microbial degradation rate is water availability in a sense that moisture fluctuations of microbial bed would cause unsteady state condition. Microorganisms die and lose their activity as the moisture content of the bed reduces in a gradual manner. This action is

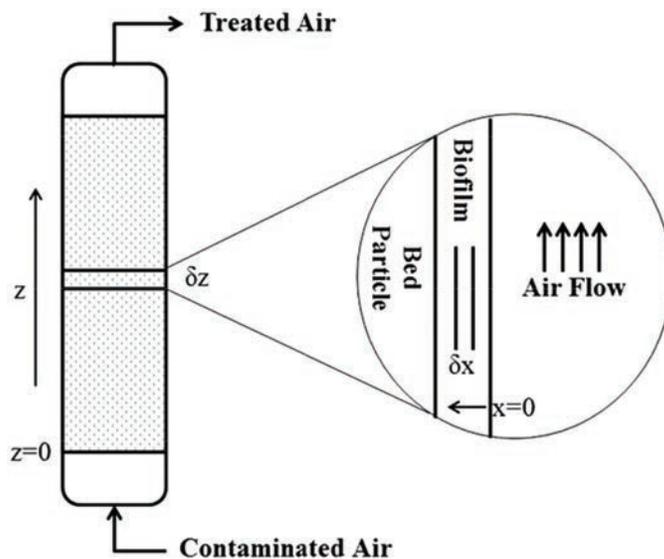


Figure 1 Schematic of a biofilter and mechanisms inside an element.

followed by reducing the performance of the biofilter which would eventually discontinue the removal of contaminant within. Thus, the moisture content of bed can be introduced as the most important regulating factor that should be controlled for the system optimum performance [2]. One of the solutions proposed in recent years to overcome the drawbacks of bed drying is applying super absorbents. The structure of water super absorbents, based on 'low cross-linked hydrophilic polymers' elongates absorbing ability and water storage time [3]. By adding these compounds to the bed, higher volume of water and minerals are observed leading to a gradual release of it in long periods.

From an industrial viewpoint, modelling of biofiltration is a necessary step if scaling-up and prediction of its performance is sought. According to the available literature, there exist two prediction methods: the mechanistic and Artificial intelligence (AI). Many attempts have been and are being made in modelling biofiltration through the mechanistic method beginning early 80s.

The trends in modelling are modified by introducing new terms like: kinetic models of Monod-type substrate inhibition [4], dispersion of gas phase [5], adsorption on solid phase [6], bed drying [7] and drying effects [8] etc. to better describe the mechanisms involved in the biofilter. Consequently, the parameters must be measured precisely through gradual progression of mathematical modelling. There exist a considerable number of models which described the experimental results in a successive manner, while there exists no comprehensive model where the most typical processes in biofiltration are applied.

A branch in computer science with an extensive growth is the AI with the ability of solving complex problems in different science areas such as 'weather forecasting problem' [9], 'vehicles autopilot systems' [10] etc. In biofiltration modelling through AI tools computational load is reduced with no need in parameter measurements. There exist few studies on biofiltration performance estimation where artificial neural network (ANN) is applied. Elias et al. [11] applied MLP (multi-layer perceptron with topology 2-2-1) neural network to predict removal efficiency (RE) in a biofiltration of polluted air treating hydrogen sulphide, Ibarra-Berastegi et al. [12] compared the two MLP and Multiple Linear Regression (MLR) methods in a biofilter that eliminates hydrogen sulphide and it is revealed that MLP (2-2-1) model outperforms the MLR. Rene et al. [13] proposed an (ANN) through aback propagation algorithm with 2 layers (topology of 4-4-2). The model is able to effective prediction of RE and elimination capacity (EC) in a hydrogen

sulphide biofiltration. The same authors [14] adopted the method for predicting and modelling RE in immobilized-cell biofiltration treating ammonia. Chairez et al. [15] applied the differential neural network (carbon dioxide production and pressure drop as input data) and designed an observer to predict EC of toluene vapors in a fungal biofilter. This observer was successfully applied for the variations in reaction and was considered as a practical tool for on-line EC. An error back propagation with momentum multilayer neural network (topology 2–4–1) is applied by Rene et al. and Ravi and Philip to predict RE of the biofilter (with the concentration and unit flow as the input variables) [16, 17]. A feed forward multilayer neural network (topology 2–10–1) was presented by Zamir et al. [18] (with temperature and ILR as input variables). Deshmukh et al. [19] compared the Radial Basis Function Neural Network (RBFN) and response surface methodology for prediction and performance optimization of a biofilter system treating toluene and revealed the superior ability of RBFN for approximate higher degree of non-linearity that was between input and output variables. Rene et al. [20] applied back propagation neural network to predict the performance parameter measured by RE with the input parameters of unit flow and inlet concentrations.

Attempt is made here to develop a mechanistic model and neuro-fuzzy approach to predict dynamic performance of the hexane biofiltration system by applying water super absorbents. In this process, after moistening stops the inlet air dries parts of the bed. As a result, the outlet concentration of the pollutant increases in a gradual manner allowing the prediction to be made. For the first time, in this context a comparison is made between two approaches in order to assess their modelling capabilities.

2 Material and Method

2.1 Adaptive Neuro-Fuzzy Inference System

The ANFIS is applied in both the ANN and FIS. ANFIS is based on Takagi–Sugeno fuzzy inference system where learning algorithm of artificial neural algorithm is applied to approximate nonlinear functions [21]. It is developed in the 1993 by Jang [22].

The subtractive clustering algorithm is practical and commonly applied approach in ANFIS networks synthesis, which estimates the cluster number and its location in an automatic manner. In subtractive clustering algorithm, each sample point is considered as a potential cluster center.

Several applications of ANFIS are presented in various fields in [23, 24]. In addition, many applications are presented with ANFIS for time series prediction [25–27]. An ANFIS is designed for earlier kick detection in oil wells through measurable drilling parameters [28, 29].

The number of clusters and each cluster location is estimated through the subtractive clustering (SC) algorithm [22, 30], where, each data point is considered as a potential cluster center. Cluster estimation is obtained through the method adopted to initialize ANFIS through the number of cluster centers in order to generate membership functions of ANFIS.

2.2 Gravitational Search Algorithm

Gravitational Search Algorithm(GSA) is a new heuristic search algorithm based on Newtonian laws of gravity and motion [31] and is applied in many scientific applications like image processing [29], filter modeling [32] etc. The optimal solution is yield through agents named masses. The masses move in the search space subject to Newtonian laws of gravity and motion [31]. The position of the i^{th} mass is determined as follows:

$$X_i = (x_i^1, \dots, x_i^d, \dots, x_i^n) \quad i = 1, 2, \dots, S \quad (1)$$

and

$$q_i(t) = \frac{fit_i(t) - worst(t)}{best(t) - worst(t)} \quad (2)$$

$worst(t)$ and $best(t)$ are defined through Equations (3 and 4):

$$worst(t) = \max_{j \in \{1, \dots, s\}} fit_j(t) \quad (3)$$

$$best(t) = \min_{j \in \{1, \dots, s\}} fit_j(t) \quad (4)$$

also,

$$M_i(t) = \frac{q_i(t)}{\sum_{j=1}^s q_j(t)} \quad (5)$$

To determine each agent’s acceleration value, the total forces from a set of heavier masses on the agent should be computed through the law of gravity, Equation (6):

$$F_i^d(t) = \sum_{j \in \{k_{best}, j^1\}} rand_j G(t) \frac{M_j(t) M_i(t)}{R_{ij}(t) + \varepsilon} (x_j^d(t) - x_i^d(t)) \quad (6)$$

Next, each agent's acceleration is calculated through Equation (7):

$$a_i^d(t) = \frac{F_i^d(t)}{M_i(t)} = \sum_{j \hat{I}kbest, j^1i} rand_j G(t) \frac{M_j(t)}{R_{ij}(t) + \varepsilon} (x_j^d(t) - x_i^d(t)) \quad (7)$$

then, the next velocity of an agent is calculated as a random coefficient of its current velocity plus its acceleration Equation (8):

$$v_i^d(t+1) = rand_i \times v_i^d(t) + a_i^d(t) \quad (8)$$

and finally, its position is computed through Equation (9):

$$x_i^d(t+1) = x_i^d(t) + v_i^d(t+1) \quad (9)$$

and $R_{ij}(t) = \|X_i(t), X_j(t)\|_2$.

The gravitational constant decreases by time:

$$G(t) = G(G_0, t) \quad (10)$$

2.3 Mechanistical Model Development

A mechanistic model is developed through mass balance to predict variations in outlet concentration of the hexane biofiltration system through water super absorbent. When moistening of the bed is stopped, the unsteady state condition governs the biofilter, that is, a gradual increase in water evaporation in the bed.

The mass transfer equations of contaminant and moisture content for such system(s) are governed within the differential element in order to develop this model. Elements contain both the gas and biofilm phases Figure 2. The z and x coordinates are considered for the gas and biofilm phases, respectively. Biofilm formed on the bed particles contains consortia of micro organisms active in pollutants' biodegradation. This phenomenon together with diffusion rate of contaminants into biofilm are considered as the limitations in biofiltration.

The focus here is to consider the terms of moisture content and axial dispersion in mass balance equations. A pattern for moisture depletion is followed in this modeling procedure which influences some of the terms like bed porosity and surface area of particles. The equations yield here are discretized through the finite volume method and are to be solved numerically in MATLAB, 2010a environment.

The simplifying assumptions are introduced in order to govern the mass transfer equations:

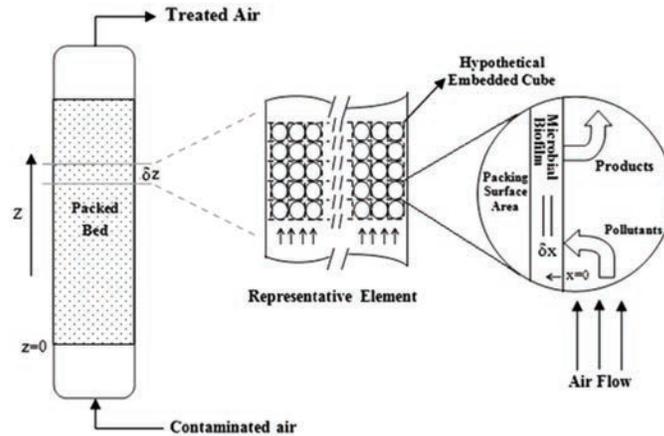


Figure 2 Schematic view of mass transfer mechanisms inside of a biofilter.

Model Assumptions

1. Due to low thickness of the biofilm in comparison with bed particles the Cartesian coordinates are considered in the equations.
2. Temperature changes during biofilter are negligible. There exists thermal equilibrium between the phases and the physical properties are constant.
3. Bed particles consist of perlite and water super absorbent which are considered spherical and non-porous with an identical average diameter in fully water saturated state.
4. Concentration changes in the radial direction is neglected and axial dispersion of gas phase in the column is considered in the equations through the dispersion coefficient.
5. The biofilm of homogeneous phase and biological reactions occur only in this phase. Its thickness and density along the biofilter are uniform and constant during the process. It only covers the surface of bed particles and does not grow on the super absorbent particles.
6. The reaction rate in the biofilm is expressed by Monod equation. The term of moisture in the reaction is independent of concentrations.
7. Resistances in gas-phase and two-phase interface are negligible, which allows the concentrations of contaminant at the interface of gas/biofilm to be in equilibrium and be defined by Henry's law.
8. Only water from the surface is exchanged with the surrounding air through bed particles regardless of the capillary effects. These particles are inert and do not adsorb the pollutant.

9. The process of water evaporation from super absorbent is modeled as evaporation from surface of a droplet with an identical diameter. The evaporation rate and transfer through the air are described by the mass transfer coefficient.
10. The porosity of bed is variable during the process. These changes occur due to withdrawal of water from the pores of perlite particles and shrinkage of super absorbent particles. The shrinkage phenomenon reduces the surface area of super absorbent particles.

Description of the Model

The following equations are obtained by establishing the mass transfer balances in both the gas and biofilm phases:

- 1) Pollutant mass balance in gas phase is:

$$\begin{aligned} \frac{\partial(\varepsilon_g C_g)}{\partial t} &= D' \frac{\partial^2 C_g}{\partial z^2} - u_g \frac{\partial C_g}{\partial z} + a D_{hex} \frac{\partial C_b}{\partial x} \Big|_{x=0} & (11) \\ Q C_g(0^-, t) &= Q C_g(0^+, t) - D' A \varepsilon_g \frac{\partial C_g(0^+, t)}{\partial z} \\ \frac{\partial C_g(L, t)}{\partial z} &= 0 \\ C_g(z, 0) &= C_{g0}(z) \end{aligned}$$

- 2) Pollutant mass balance in biofilm phase is:

$$\begin{aligned} \frac{\partial C_b}{\partial t} &= D_{hex} \frac{\partial^2 C_b}{\partial x^2} - \frac{X_v}{y_{x/s}} \frac{\nu_m C_b}{K_s + C_b} & (12) \\ C_b(0, z, t) &= \frac{C_g(z, t)}{m} \\ \frac{\partial C_b(x_n, z, t)}{\partial x} &= 0 \\ C_b(x, z, 0) &= C_{b0}(x, z) \end{aligned}$$

- 3) Moisture balance in gas phase is:

$$\begin{aligned} \frac{\partial(\varepsilon_g H_g)}{\partial t} &= D' \frac{\partial^2 H_g}{\partial z^2} - u_g \frac{\partial H_g}{\partial z} + a D_{H_2O} \frac{\partial H_b}{\partial x} \Big|_{x=0} = & (13) \\ D' \frac{\partial^2 H_g}{\partial z^2} - u_g \frac{\partial H_g}{\partial z} &+ K_c a (H^* - H_g) \end{aligned}$$

$$QH_g(0^-, t) = QH_g(0^+, t) - D'A\varepsilon_g \frac{\partial H_g(0^+, t)}{\partial z}$$

$$\frac{\partial H_g(L, t)}{\partial z} = 0$$

$$H_g(z, 0) = H_{g0}(z)$$

Two equations describing the amount of water of the bed and super absorbent applied in each one of the elements are:

$$\frac{\partial m_p}{\partial t} = -K_c a_p (H^* - H_g) \quad t = 0, m_p = m_{p0} \quad (14)$$

$$\frac{\partial m_s}{\partial t} = -K_c a_s (H^* - H_g) \quad t = 0, m_p = m_{p0} \quad (15)$$

According to the common data presented for both the perlite (bed material) and super absorbent products, water absorption is calculated to determine initial water content of the particles in the column at the beginning of unsteady state conditions. The initial water content is reduced gradually during the evaporation until use up.

The developed equations are discretized through Finite Volume Method. Modeling parameters are obtained from both the available literature or through precise calculations. Available data from a reliable source [3] are applied with parameters of hexane biofiltration literatures in order to verify this proposed model, Table 1 [33, 34].

Table 1 Model parameters of bacterial biofiltration [33, 34]

Parameter	Value	Unit	Parameter	Value	Unit
specific surface area (A_s)	2600 ^a	m^{-1}	Hexane partition coefficient in water (Henry's constant) (m_{Hex})	9.14	-
effective diffusivity of pollutant (D_{Hex})	2.58×10^{-10}	$m^2 s^{-1}$	yield coefficient of biomass on Hexane ($Y_{x/s}$)	1.314 ^c	-
dispersion coefficient (D')	1.22×10^{-4b}	$m^2 s^{-1}$	biofilm thickness (x_n)	387	μm
bed porosity (ε_g)	0.45	-	biofilm density (X_v)	9744	gm^{-3}
saturation constant (K_s)	0.02	gm^{-3}	maximum specific growth rate (v_m)	5.83×10^{-5}	h^{-1}

a) Fitted value; b) Spigno and Favari [34]; c) Calculated value.

2.4 Development of a ANFIS for Modelling Hexane Biofiltration

In this article, 71 sets of inputs-output data pairs have been applied for training and test phases. The test data set includes 15 data points (26% all of data) and the training data set is composed of 56 data points (74% all of data). During the training process, the error between real value of the target and ANFIS output is minimized. Training enables ANFIS to learn features from the training and implement them in the system rules. In the test phase, the learned system is applied on the test data set for assessment. A subtractive clustering (SC) technique is applied to formulate the ANFIS. In the SC method each data point is considered as a potential cluster center, and, based on the density of surrounding data points, a measure of likelihood where, each data point would define the cluster center, is calculated. The fitness function of GSA is chosen to be the mean square error of ANFIS structure over training data set. The GSA-SC-ANFIS generation is shown in Figure 3. The GSA parameters consist of: (for $G(t) = G_0 e^{-\alpha \frac{t}{T}}$ In Equation 10) $\alpha=20$, $G_0=100$ and $N=50$.

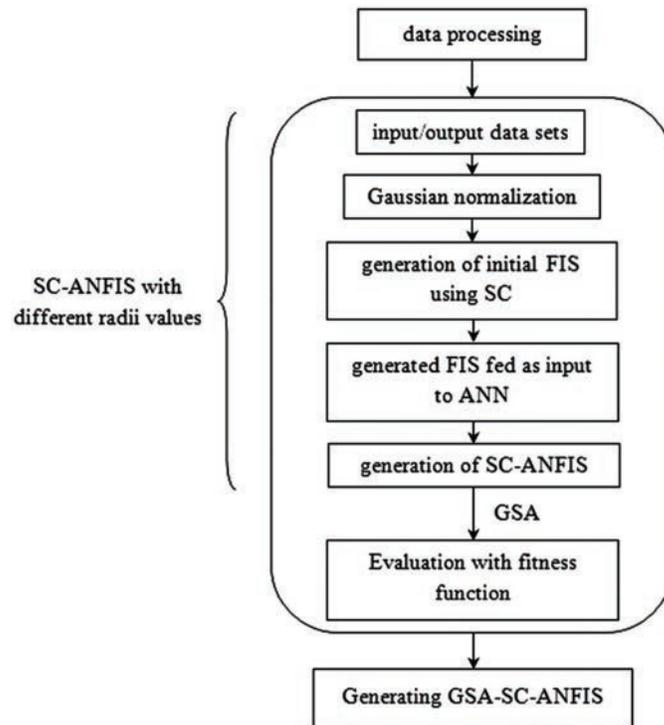


Figure 3 Flowchart of the proposed combined algorithm.

In this proposed ANFIS-based algorithm, similar to common fuzzy inference systems, the parameters are tuned during the training process in an automatic manner; hence, the membership functions could represent the nonlinear behavior of the system in a proper manner.

2.5 Error Estimation

In this study, the following two criteria are considered for comparing the two methods: Mean squared error (MSE) and coefficient of determination (R^2) which are defined through Equations 16 and 17, respectively:

$$MSE = \left(\frac{1}{n} \sum_{i=1}^n (Y(p_i) - Y(o_i))^2 \right) \times 100 \quad (16)$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^n (Y(p_i) - Y(o_i))^2}{\sum_{i=1}^n Y(o_i)^2} \right) \quad (17)$$

3 Results and Discussion

The capability of both modelling approaches in prediction of dynamic performance of the biofiltration is assessed. When bed watering stops unsteady state condition governs the biofilter. As a result of evaporation, the activity of microorganisms which degrade the pollutants decrease in a gradual manner and the outlet concentration of contaminants increases. The inlet air with low moisture content saturation dries parts of the bed and stops the microorganisms' activities.

This phenomenon is considered as ε_g in each element of the model. At this stage, each element contains a specific portion of the total available water of the biofilter and loses it with a specific rate in mass transfer. Such a decreasing trend, locally, affects ε_g . Some of the terms in the mass transfer equations, like coefficients of equations related to pollutant concentrations in both the phases, superabsorbent specific surface area (superabsorbent becomes smaller as it loses water) and mass transfer coefficient in moisture equation depend on changes inflicted on ε_g . Any change in ε_g will change these coefficients and increase the concentrations of pollutants in the elements. Since each element takes its inlet from the previous element, the effect of increasing concentration in initial elements which is then transferred to other elements is observed in the outlet. When each element loses all its water content, water drain begins in the next element this trend continues until the bed water content is evaporated completely. This increase ultimately yields to the failure of the system.

In the ANIFS method, Inlet concentration and flow rate of biofiltration experiments are applied as the inputs and the outlet concentration is selected as the output of the ANFIS. This proposed method is adopted to learn the input–output correlations according to the training data set. In the learning phase, the ANFIS, first, makes the appropriate membership functions for each input. In the sequel, the membership functions are tuned according to error correction training method applying BP algorithm. In addition, the constant parameter of the linear output functions is applied during the learning phase based on Recursive Least Square (RLS) algorithm.

The outlet concentrations of biofilter with inlet concentrations of 0.5 g/m^3 and 1 g/m^3 and 0.3 l/min flow rate which are predicted by ANFIS-based method and mechanistic model are illustrated in Figure 4. For 0.5 g/m^3 concentration, experimental data of biofiltration are gathered in arbitrary days between 37 and 60. After day 55, the two curves are set apart from each other in a gradual manner. Mechanistic modelling and ANFIS-based method have reached to inlet concentration of 0.5 g/m^3 at days 64 and 77, respectively, where, both of methods lose few data points, although it is assumed that they fairly fitted the experimental data. For 1 g/m^3 concentration, mechanistic modelling and ANFIS-based method both reach the inlet concentration at days 79 and 91,

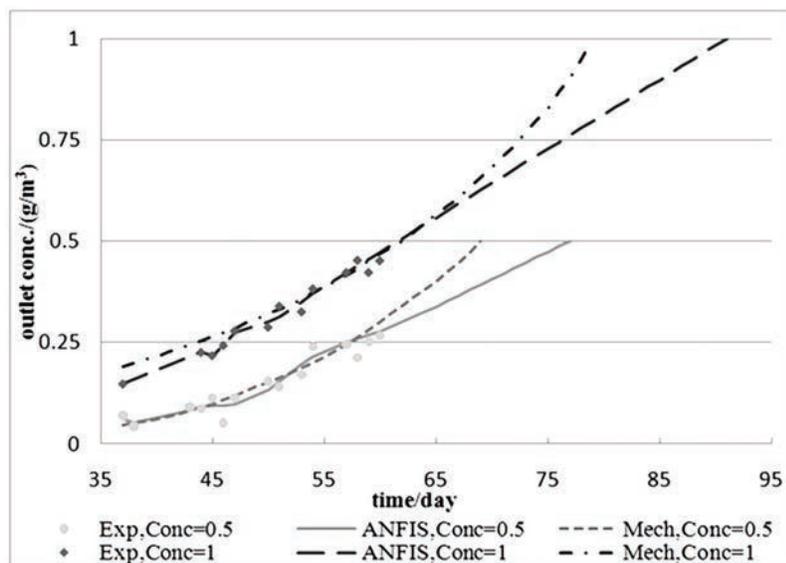


Figure 4 Prediction of outlet concentration by ANFIS-based method and mechanistic model (Inlet concentration of 0.5 g/m^3 and 1 g/m^3 with flow rate of 0.3 l/min).

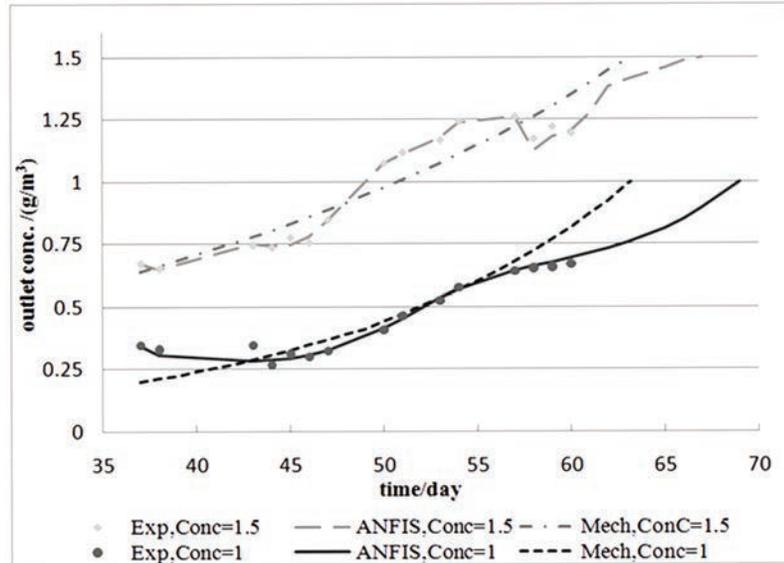


Figure 5 Prediction of outlet concentration by ANFIS-based approach and mechanistic method (Inlet concentration of 1 g/m^3 and 1.5 g/m^3 with flow rate of 0.5 l/min).

respectively. In this case, due to lack of outlier data points, the outcomes of both the models are fitted to experimental data points.

The outlet concentrations of biofilter of 1 g/m^3 and 1.5 g/m^3 with inlet concentrations and 0.5 l/min flow rate, Figure 5. Regardless of the first and the last few days, both of the obtained curves are well mapped on experimental data. Moreover, 1.5 g/m^3 inlet concentration is reached at days 63 and 67 by mechanistic modelling and ANFIS-based method, respectively.

The outlet concentrations of biofilter with 1 g/m^3 inlet concentration and 0.7 l/min flow rate predicted by ANFIS-based method and mechanistic model, Figure 6. The 1 g/m^3 inlet concentration is reached at days 56 and 76 through mechanistic modelling and ANFIS-based method, respectively. In this case, mechanistic method is not able to model biofiltration performance in a proper manner. The main reason might be that most of parameters like diffusion coefficient of pollutant are considered constant, while they change due to higher air flow rate in a rapid manner.

The results here indicate that more precise predicting capability of ANFIS-based method can be introduced as a new powerful modelling approach. In general, this approach lacks the ability to describe the system and does not have any ideas regarding mechanisms but it provides an estimation of results

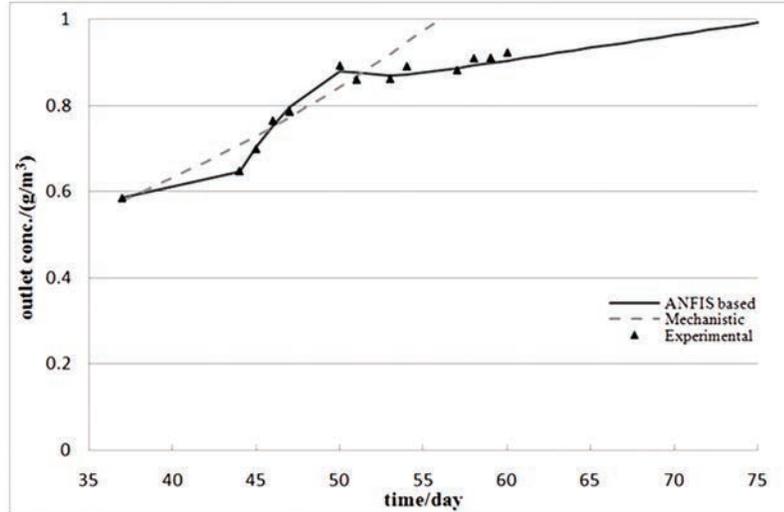


Figure 6 Prediction of outlet concentration by ANFIS-based approach and mechanistic method (Inlet concentration of 1 g/m^3 and flow rate of 0.7 l/min).

regardless of the solution complexities. Despite the fact that mathematical modelling which is case-specific and endures parameters measurements, ANFIS-based modelling has the potential to generalize most of the biofiltration systems subject to favourable conditions. Though new efforts for mechanistic modelling contribute to better understanding of heat and mass transfer mechanisms involved in biofiltration, they assist scaling up and optimizing of such systems.

The MSE and R^2 over train and test data achieved through ANFIS-based algorithm and mechanistic methods are tabulated in Table 2. The proper clusters' radii to obtain the best results are set through GSA in order to accomplish the least mean square error over training data. It could be deduced that both the methods could precisely predict outlet concentrations over test

Table 2 MSE and R^2 over test and train data

		GSA-SC-ANFIS	Mechanistic
MSE	test data	0.028%	0.499%
	train data	0.0003%	0.400%
R^2	test data	0.998	0.992
	train data	0.999	0.989

and train data. However, ANFIS-based method yields more accurate prediction when compared to its counterparts. It should be noted that there exist few outlier experimental data points which keep the error rate low in both the models.

4 Conclusion

Modelling of biofiltration is a valuable tool for better understanding the system and prediction of its performance. In this article, two approaches of modelling are presented to predict variations in outlet concentration of a hexane biofiltration system subject to unsteady state conditions by applying water super absorbent for water supply improvement. To get a better view of the methods, the ANFIS-based approach is compared with the mechanistic model. The obtained results reveal the high strength of both approaches in predicting the outlet concentrations however the higher accuracy is achieved by ANFIS-based method. While ANFIS-based has the potential to generalize most of the biofiltration systems, the mechanistic modelling has the ability to describe a system and provide new ideas on mechanisms.

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