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Mathematical Modeling and Parameters Optimization of the Degradation of Acrylonitrile in Biofilters

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ABSTRACT

The removal of Acrylonitrile (AN) from waste gas streams using biological methods, due to their better performance, has recently gained more attraction. The purpose of this research is modeling the AN removal by a bio-filter. The validation of the model is done by using the experimental data of a bench-scale bio-filter bed column including yard waste compost and shredded hard plastics and thickened municipal activated sludge. In this work the kinetics of the biodegradation of Acrylonitrile is first investigated. Then equations of the biofilm and air are obtained at a steady state and constant temperature. The unknown parameters of the model are determined by the least square optimization method along with solving the model equations using MATLAB. For inlet concentrations less than 1 g/m^3 the model results show reasonable similarities to the experimental data. The effect of various parameters on the bio-filter performance is evaluated. The Peclet number, biofilm thickness and biomass concentration are the most important parameters. The proposed model can be useful for design purposes.

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1. Introduction

Acrylonitrile (AN), a volatile organic compound mostly emitted from chemical and petrochemical industrial processes, is the third in the list of toxic and hazardous contaminants of EPA [1, 2]. In recent years the bio-filtration technology, because of its economical and environmental benefits, has been used more than other methods for removing the unwanted compounds from waste gas [3-5].

Bio-filters include packing material (e.g. peat, compost) on which micro-organisms grow as biofilms. Waste gases are transferred through the packed bed to be purified. Contaminants are conveyed from the gas

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phase to the biofilm in which they diffuse and undergo the aerobic biological degradation. During the process sufficient levels of moisture, oxygen and nutrients required for the biomass activation should be maintained [6].

During the past three decades, several mathematical models have been described the different phenomena of the bio-filtration processes [7, 8]. The first model was proposed by Ottengraf and Van den Oever [9], which included the simple zero or first order model for the degradation of a substrate in a biofilm and plug flow assumption for the gas stream. Ottengraf's model was used as the basis for more complicated ones proposed later. Hodge and Devinny developed the kinetic model and used the Haldane type model which was comprised of Michaelis–Menton growth equation including the inhibition term [10]. Shareefdeen et al. [11], Alonso and Suidan [12] and Deshusses et al. [13] added the oxygen inhibition term and Baquerizo et al. [14] used a comprehensive model including expression for the nutrient limiting effect. In addition to kinetic equations they also corrected the gas mixing model.

Shareefdeen et al. [11], Spigno et al. [6], Baquerizo et al. [14] and alvares et al. [15] removed the plug flow assumption for gas stream and incorporated a dispersion factor in modeling the gas mixing in the bio-filter.

Existing models appear to be sufficient for the mass transfer in the air and the biofilm phase with a simple combination. The major problem in the mathematical modeling of bio-filters is determining model parameters. Since the direct measurement and accurate determination of parameters are not possible, the reverse modeling is a way to solve this problem using valid experimental data about the removal of the substrate in a bio-filter with the help of a mathematical model during the model validation stage [3]. For the inverse modeling, we need an efficient optimization technique. Kiranmai et al. [16] used the differential evolution method to determine the bio-kinetics in a fixed-film reactor modeling equations; Bhat et al. [3] developed it for the efficient estimation of parameters in bio-filter modeling and Rene et al. [17] used neural networks models to predict the dynamics of the bioreactor performance.

In this research, in addition to modeling the bio-filter an experimental work of the removal of acrylonitrile is used to estimate unknown parameters in the bio-filter modelling. The Existing models mentioned above have used materials other than acrylonitrile to validate them. Given the fact that acrylonitrile is an important contaminant, the importance of this work becomes clear.

The main purpose of this research is to propose a simple model to predict the performance of the acrylonitrile bio-filter and determine the unknown parameters of the model with optimization. The first goal was the validation of the model using the experimental data of a bench-scale bio-filter bed column and investigation of the kinetics of the biodegradation of acrylonitrile. The second goal was the determination of the unknown parameters of the model by the least square optimization method along with solving the model equations using MATLAB. According to our studies, the model suggested in here and based on the method described in this article for Acrylonitrile has not been presented in depth in any other research so far which shows the novelty of the present research.

2. Materials and methods

The system modeled in this research is a bench-scale bio-filter, which Dehghanzadeh et al. [18] used to remove acrylonitrile vapor from waste gas streams. Its main features are listed in Table 1.

The operation was done at the atmospheric pressure and temperature of 30 ± 1 °C. During the operation time the humidity of the bed material was maintained at 60-65 %. The bed consisted of yard waste compost, shredded hard plastics and thickened municipal activated sludge [18].

Figure 1 shows the experimental set up. To sample the gas composition four ports were embedded along the bio-filter bed.

Table 1
Parameters of the experimental set-up and operating condition [18].

Parameter	Value
Total bed volume, m^3	0.008
Bed column height, m	1.2
Surface area, m^2	0.05
Bed porosity, %	54
Inlet acrylonitrile concentration, g/m^3	0.4-2.6
Gas velocity, m/s	0.003-0.04
Operating temperature °C	30

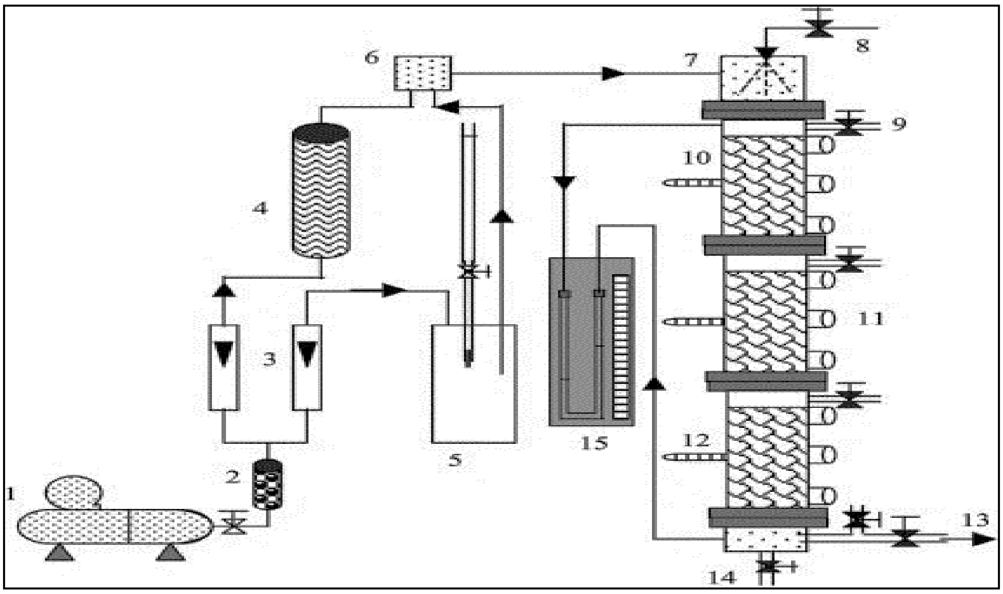

Figure 1. Schematic of the bio-filter system: 1-compressor, 2-carbon filter, 3- rotameter, 4-humidifier, 5-pollutant vessel with Acrylonitrile injector, 6-mixing chamber, 7-gas inlet, 8- nutrient inlet, 9-gas sampling port, 10- bio-filter bed, 11-bed sampling port, 12- thermometer,13- gas outlet, 14- leachate discharge,15-manometer [18].

3. Mathematical modeling

The basis of mathematical model is the principal mechanisms of bio-filtration like the contaminant transfer from gas phase to the liquid phase, the diffusion into the biofilm, and the biodegradation reaction. The basis of biodegradation kinetics is a Haldane-type expression, which considers the self-inhibition effect of the substrate.

The assumptions of the model are:

1. The mass transfer and biological degradation are assumed to be at steady states.
2. The operating pressure and temperature are constant.
3. The biofilm is assumed to be flat due to its less thickness relatively to the main curvature of the solid particles, so model equations are derived for a planar geometry.
4. The physical properties such as the biomass density and biofilm thickness are constant throughout the filter bed. The thickness of the biofilm varies with the variation of the inlet load and the relationship is considered as below [3]:

$$\delta = C_1 + C_2 L \quad (1)$$

where C_1 is considered 30 μm as the initial value and changes by adjusting C_2 during optimization.
5. The solid particles and biofilm do not adsorb the contaminant.
6. The oxygen or nutrient limitation does not occur.
7. Acrylonitrile is consumed to be in equilibrium at the bio-layer-air interface and expressed by Henry's law:

$$C_b = \frac{C_g}{m} \quad (2)$$

The distribution coefficient (m) is the half amount of that of when the bio-layer is made of water only.
8. The gas flow is assumed to be dispersed along the bio-filter bed.
9. The diffusion resistance controls the mass transfer of the anion in the biofilm. Fick's law has used to represent the diffusion of the substance into the biofilm. The empirical equation, developed by Fan et al., is used to estimate the diffusion coefficients of the biofilm [19]. It relates the diffusion coefficient in the biofilm to the diffusion coefficient measured in water and the total biomass density in the biofilm (X in g/l):

$$D_b = D_W \left[1 - \frac{0.43 X_b^{0.92}}{(11.19 + 0.27 X_b^{0.92})} \right] \quad (3)$$

3.1. Equations

3.1.1. Kinetic equation

Considering the substrate inhibition effect, the degradation kinetics of acrylonitrile is expressed by Haldane type model:

$$EC_{AN} = EC_{max} \frac{C_{ln}}{C_{ln} + K_s + C_{ln}^2 / K_I} \quad (4)$$

EC_{max} (g/m^3 h) is the maximal EC, C_{ln} (g/m^3) and represents the logarithmic average of the inlet and outlet concentrations of pollutants in the gas phase; K_s (g/m^3) is the Monod half saturation constant and K_I (g/m^3) shows the inhibition constant for the Haldane type model.

3.1.2. Mass balance in biofilm

The concentration of acrylonitrile in a controlled volume of the biofilm changes with the acrylonitrile diffusion and biological reaction rate (r_s).

Fick's law is used to represent the diffusion of the pollutant into the biofilm:

$$N_{b,AN} = -D_b \frac{dC_b}{dx} \quad (5)$$

Therefore, the mass balance in the biofilm is included in the following equation:

$$D_b \frac{d^2 C_b}{dx^2} - r_s = 0 \quad (6)$$

The relationship between r_s and EC is:

$$r_s = ec \times \frac{X_b}{X_r}, \quad X_r = A_s^* \delta X_b \quad (7)$$

Using Henry's law, the kinetic model was obtained as a function of the concentration of AN in the biofilm:

$$EC_{AN} = EC_{max} \frac{C_b}{C_b + K_s + C_b^2 / K_I} \quad (8)$$

With the combination of the above equations the overall equation was obtained:

$$D_b \frac{d^2C_b}{dx^2} - \frac{EC_{max} C_b}{C_b + K_s + C_b^2 / K_I} \left(\frac{X_b}{X_r}\right) = 0 \quad (9)$$

To solve the above equation, two boundary conditions are needed:

$$C_b(x = 0) = \frac{C_g}{m} \quad (10)$$

$$\left.\frac{dC_b}{dx}\right|_{(x=\delta)} = 0 \quad (11)$$

where x = δ is the effective thickness and x = 0 is the biofilm surface.

3.1.3. Mass balance in gas phase

The concentration of acrylonitrile in the gas phase changes through the dispersion, convection, and diffusion at the biofilm surface. The overall mass balance equation is:

$$-u_g \frac{dC_g}{dz} + \varepsilon D \frac{d^2C_g}{dz^2} + D_b A_s^* \left.\frac{dC_b}{dx}\right|_{x=0} = 0 \quad (12)$$

where D is the dispersion coefficient and calculated by experimental measurements [20] or the approximation of Peclet number through the following correlation (which has been done in this research):

$$D = \frac{u_g h}{\varepsilon \times pe} \quad (13)$$

The boundary conditions are:

$$\frac{dC_g}{dz} = 0 \qquad z = h \quad (14)$$

$$C_g = C_{gin} \qquad z = 0 \quad (15)$$

3.2. Model parameters

Table 2 shows the parameters and their values needed to solve the model equations. The kinetic parameters K_s, EC_{max} and K_I were estimated by fitting the model to experimental data (C_b, EC_{max}). We used the Wilke-Chang equation to calculate the diffusivity coefficient of acrylonitrile in water [21] and the Wilke- Lee equation to calculate the diffusivity coefficient of acrylonitrile in air [22]; the partition coefficient of the gas-biofilm was considered as the half of the value of that of air-water [22].

The biomass density in the reactor was calculated by equation (7) and the values of the last four parameters were obtained with optimization.

3.3. Model solution

MATLAB®9 software was used to solve the model equations. The equation in the bio-layer was solved using the shooting method that has been developed in MATLAB based on a Runge-Kutta method and the gas phase equation was solved analytically. The two equations were solved simultaneously with the discretization of the spatial domain of the height of the reactor column. The optimization was carried out along with the solution of the equations by the least mean square error (LMS) algorithm to determine the unknown parameters of the model.

Table 2
Model parameters.

Parameter	Unit	Value	Reference
Maximum elimination capacity, (EC_{max})	g/m^3 h	230	Curve
Monod half saturation constant, (K_s)	g/m^3	0.8886	fitting
Inhibition constant, (K_I)	g/m^3	4.245	
Acrylonitrile diffusivity in water, (D_W)	m^2/s	1.37986e-10	[20]
Acrylonitrile diffusivity in air, (D_g)	m^2/s	1.1413e-5	[21]
Air–water acrylonitrile partition coefficient, (m)	-	0.0040751	[22]
Porosity, (ε)	-	0.54	[18]
Biomass density in reactor, (X_r)	kg/m^3	500	This work
Specific surface area, (A_s)	m^{-2}	120	[6, 23, 24]
Thickness biofilm, (δ)	Mμ	30+0.02L*	[3, 6]
Biomass density in biofilm, (X_b)	kg/m^3	120	[6, 25]
Peclet number, (Pe)	-	3	[20]

*L: Acrylonitrile mass loading rate

4. Removal efficiency

The removal efficiency (RE) is the fraction of the pollutant removed by the bio-filter performance:

$$RE = 100 \times \frac{C_{g,in} - C_{g,out}}{C_{in}} \quad (16)$$

EC is the mass of the pollutant removed per unit volume of the bio-filter material per the unit time:

$$EC = Q \times \frac{C_{g,in} - C_{g,out}}{V_f} \quad (17)$$

The EC can be also expressed as:

$$EC = L \times \frac{RE}{100} \quad (18)$$

where L (mass loading rate) is the value of the inlet pollutant to the bio-filter per the unit volume of bed per the unit time. The EC is a normalized term of the bed volume and flow rate and can be used to compare the performance of bio-filters.

5. Results and discussion

5.1. Model validation

The validation of this model was done using experimental data from a bench-scale bio-filter which Dehghanzadeh et al. [18] used to remove acrylonitrile vapor from waste gas streams. The main accessible data were the concentrations of the inlet and outlet AN, gas flow rate and velocity, experimental set up features and operating conditions which are listed in Table 1.

5.1.1. Kinetic model

The Haldane type kinetic model parameters K_s, EC_{max} and K_I were estimated by fitting the model to experimental data (of C_{gin} , EC_{exp}). The values obtained are 0.869g/m^3, 230 g/m^3 h and 4.25 g/m^3 respectively with the value of 0.99 for R^2.

Figure 2 shows the elimination capacity of the bio-filter as a function of the logarithmic average of the concentration of the inlet AN. The difference between the model prediction and the experimental data is acceptable. Also it can be observed that at low concentrations, the elimination capacity increases with the increase in the concentration of the inlet AN until the maximum amount reaches a critical concentration (2 g/m^3).

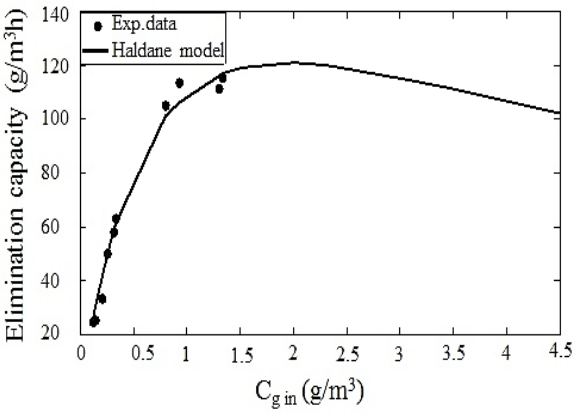

Figure 2. The relationship between the concentration of the inlet AN and elimination capacity.

After this point the elimination capacity has no increase and begins to decrease with the increase in the concentration of the inlet. The reason is the limited capacity of microorganisms in consuming the substrate. As it can be seen in Figure 2, the further amount of acrylonitrile becomes inhibitory and the elimination capacity falls.

It is worth to note that the inhibiting concentration varies for different substrates and operating conditions. It should be said that in general the elimination capacity strongly depends on the amount of the organic compounds of the filter bed. Also it's affected by the residence time. When the residence time increases, there is enough time for AN to transfer and diffuse into the biofilm. Figure 3 shows the elimination capacity as a function of the mass loading rate. As it can be observed, with the increase in the amount of the organic compounds to about 150 gr/m^3 h the elimination capacity increases gradually and linearly. For greater values the growth of the elimination capacity is slow and the maximum value is about 120 g/m^3 h. For values greater than the critical point, acrylonitrile becomes inhibitory and the elimination capacity falls.

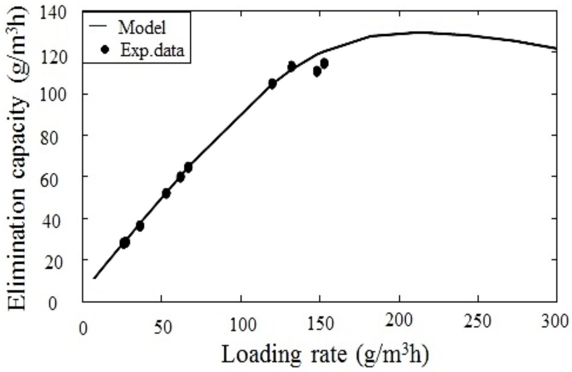

Figure 3. The relationship between the mass loading rate of the gas stream and the elimination capacity of AN.

5.1.2. General model

The values of the unknown parameters of the model were determined with optimization using the experimental data set of 10 points (of C_g, EC_{exp}). Then we used the model to evaluate the bio-filter performance at different conditions. In Figure 4, we can observe the model results for all the 10 data sets and their comparison to the measured values. It shows good agreement and the maximum error is 4.6 %.

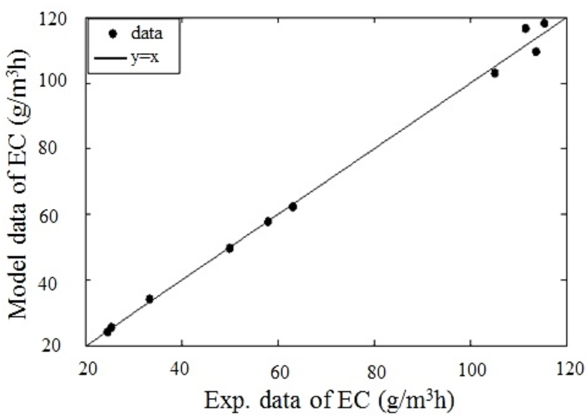

Figure 4. Elimination capacity of the bio-filter at the exit (comparison of the model prediction (line) and experimental data (points)).

Figure 5 shows the concentration profile of acrylonitrile in the gas phase over the bio-filter height. Points are the experimental data and the line is the model prediction. As it can be seen, the starting part of the curve is linear. It means that at the beginning of the bio-filter the concentration of the AN varies linearly but then it changes to be exponential and at the end part it is almost a horizontal line and the concentration doesn't change. At the inlet concentration of 0.43 g/m^3 there is a very good agreement between experimental data and model results. At the inlet concentration of 1.263 g/m^3 the concentration profiles of both the model and experimental data are parallel. At z = 0.4 m some deviation can be observed.

The humidity changes, high concentration of the contaminant in the biofilm, and short contact time have the greatest impact on the first quarter of the bio-filter. However, it can be said that due to the microorganisms having problems adapting to the condition, the rate of the degradation is still low. As we move further over the bio-filter height (at about the second part of the bio-filter), adaptation occurs and the degradation rate increases; this is more obvious for high inlet concentrations because a high amount of substrate is accessible. At low inlet concentrations, even after the adaptation, the consumption rate is low because a less amount of the substrate is accessible. On the other hand, the water and nutrient contents are not the same at different locations of the bio-filter. Also different concentrations of the inlet AN affect the microorganism activity. All these factors cannot be considered in modeling; as the consequence, the deviation of the model from the experimental data is expected.

On the whole it can be concluded that the proposed model is accurate for the inlet concentrations below 1 g/m^3.

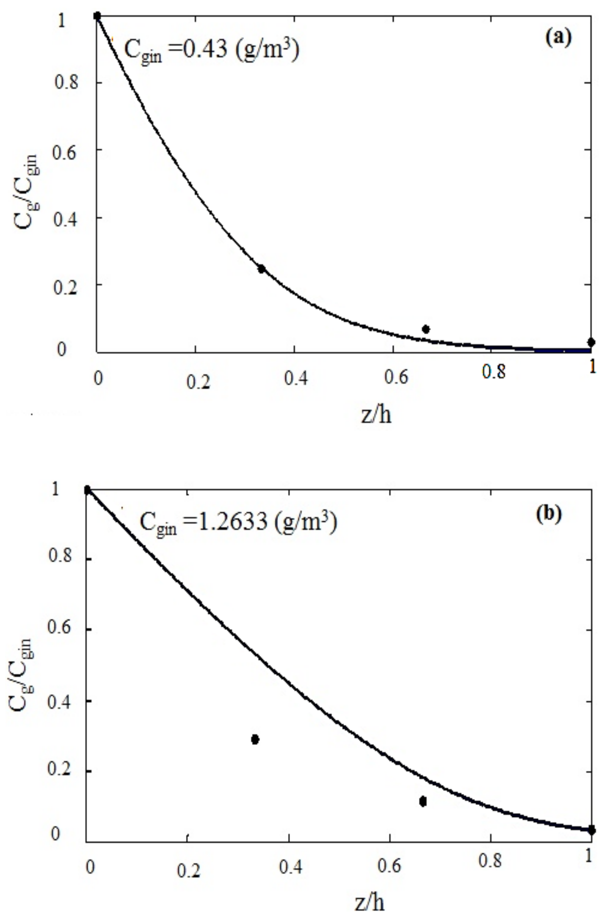

Figure 5. Concentration profile of acrylonitrile in the gas phase over the bio-filter height, the comparison of the model prediction (curve) and experimental data (points); (a) C_{gin} = 0.43 g/m^3 and (b) C_{gin}= 1.263 g/m^3.

5.2. Concentration profile of AN in the biofilm

The concentration of AN in the biofilm depends on the concentration of AN in the gas phase, diffusivity of AN in the biofilm, partition coefficient of the gas- biofilm, physico–chemical properties, and degradation rate of AN.

Figure 6 (a) and (b) show the concentration profile of AN in the biofilm for different concentrations of the inlet AN and different heights of the bio-filter respectively. As it can be observed, at the top of the bio-filter where the concentration of AN in the gas phase is high the concentration of AN in the biofilm is also high, and at the bottom of the bio-filter it is low. On the other hand, the curves in both figures are almost horizontal; furthermore, the concentration of AN in the biofilm has no significant variation and can be assumed constant. It can be concluded that in the bio-filtration of AN there is no diffusion or transfer limitation in the biofilm and the degradation rate is controlled by the reaction rate only. It is worth to mention that some other factors such as the oxygen and nutrient limitation can also affect the degradation process in the bio-filter. In this work, it is assumed that there are excess oxygen and sufficient amount of nutrient for the micro-organisms to be active. In bio-filters the filter bed is comprised of natural materials such as peat and compost that have the sufficient nutrient which is needed for the micro-organisms activity. Also it can be obtained during the operation. But further investigation should be done to show the effect of the oxygen limitation.

5.3. Sensitivity analysis

Sensitivity analysis was done to determine the impact of different parameters on the bio-filter performance. In this research, the relative sensitivities of the parameters at optimum point were calculated which is described as below:

$$S_j^{Cgout} = (\Delta C_{gout} / \Delta j) \times (j^{opt} / C_{gout}^{opt}) \qquad (19)$$

where j^{opt} is the optimized amount of parameter, C_{gout}^{opt} is the outlet concentration in the bio-filter, and S_j^{Cgout} is the relative sensitivity.

The purpose of this analysis is to determine the most important parameters which have significant effects on the bio-filter performance. Furthermore, in order to avoid large deviation of the model result from real data, the amount of these parameters should be determined accurately. Also for improving the bio-filter performance in the experimental operation, these parameters should be watched closely.

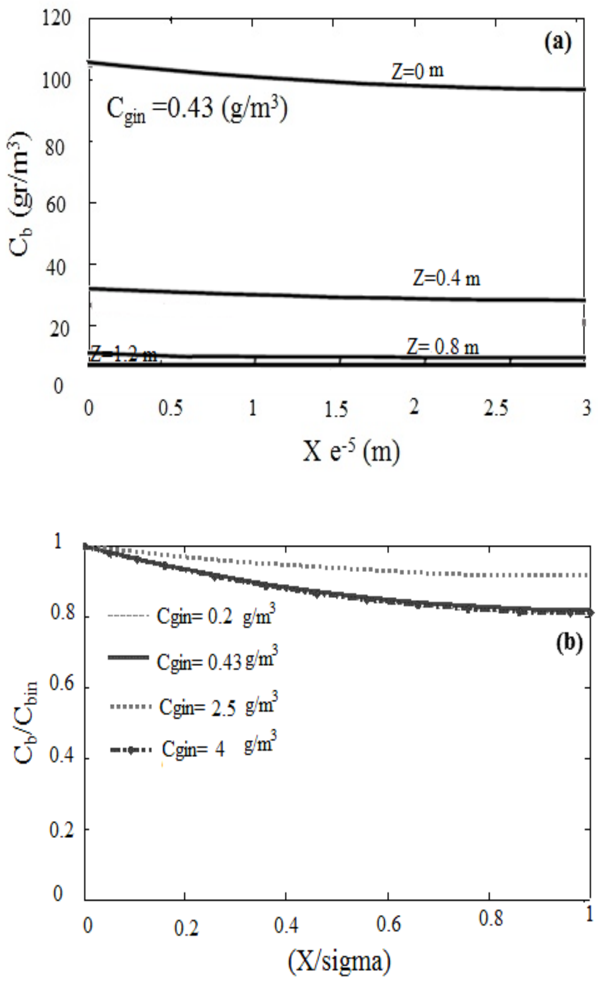

Figure 6. AN concentration profile in biofilm, (a) for different location at C_{gin} = 0.43 g/m³, (b) for different inlet concentration at z = 0.4 m.

The relative sensitivities of the parameters in this research are listed in Table 3. The results show that the Peclet number, biofilm thickness, and biomass density are the most sensitive and so the most important parameters in the bio-filtration of acrylonitrile.

Table 3
Relative sensitivity of model parameters.

Parameter	Relative sensitivity
Biofilm thickness	8.76
Specific surface area	6.1
Biomass density in biofilm	8.34
Maximum degradation rate	7.46
Peclet number	8.86
Half saturated constant	2.99
Inhibition constant	0.51

Figure 7 (a) and (b) show the removal efficiency of the bio-filter versus the Peclet number for different densities and biofilm thickness respectively.

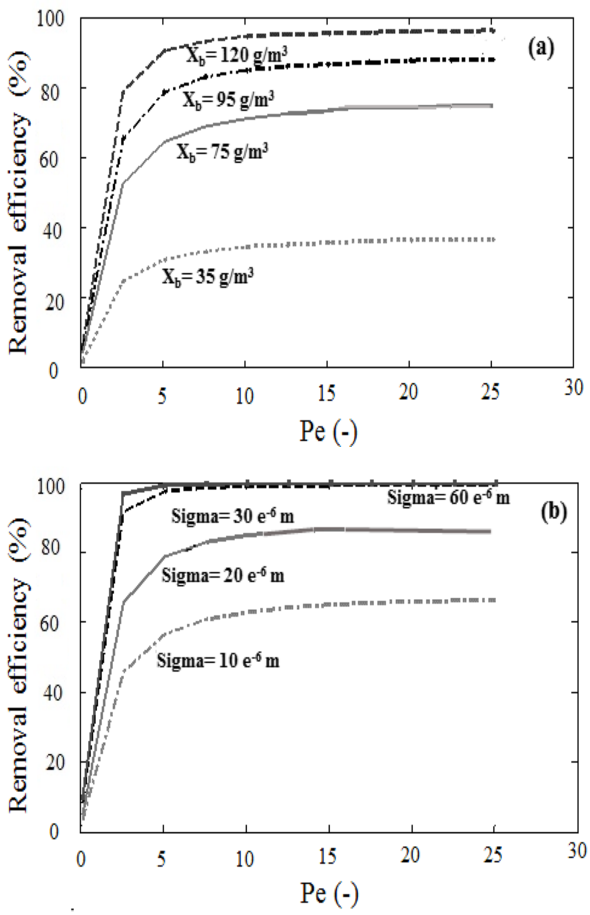

Figure 7. Removal efficiency of the bio-filter vs the Peclet number, (a) for different densities, (b) for different biofilm thicknesses.

As it can be seen the sensitivity of the Peclet number (of 5.03) used in this research is high but for higher amounts the sensitivity decreases. Also the removal efficiency increases with the increase in the biomass density (Figure 7(a)) and biofilm thickness (Figure 7(b)).

As we know the biofilm has a limited active thickness and above this amount the biofilm is inactive. In this research the effective layer was considered.

6. Conclusions

In this research, a simple model is proposed to evaluate the bio-filter performance. The Haldane type kinetic model parameters K_S, EC_{max} and K_I were estimated by fitting the model to experimental data. The model equations along with the experimental data set of 10 points (of C_g, EC_{exp}) were used to optimize the values of the unknown parameters. The values obtained are 0.869 g/m^3, 230 g/m^3 h and 4.25 g/m^3 with the value of 0.99 for R^2. The model then was used to evaluate the bio-filter performance. The difference between model prediction and the experimental data is acceptable. It can be observed that at low concentrations, increasing the concentration of the inlet AN increases the elimination capacity, until the maximum amount at a critical concentration is reached (2 g/m^3). After this point the elimination capacity has no increase and begins to increase with the increase in the inlet concentration.

The results showed that the proposed model is accurate for the inlet concentrations below 1 g/m^3.

Moreover, the sensitivity analysis was done to determine the impact of different parameters on the bio-filter performance. The results show that the Peclet number, biofilm thickness and biomass density are the most important parameters in the bio-filtration of acrylonitrile. These results can be useful for designing purposes in the future.

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Nomenclature

A_s^*	specific surface area per unit reactor volume [m^{-1}].
C_g	Acrylonitrile concentration in the gas phase [g/m^3].
C_b	Acrylonitrile concentration in biofilm [g/m^3].
D_w	Acrylonitrile diffusion coefficient in water [m^2/s].
H	the bed height [m].
K_I	inhibition constant [g/m^3].
K_s	Monod constant [g/m^3].
m	air–water distribution coefficient for Acrylonitrile.
Pe	Peclet number.
Q	volumetric flow rate [$m^3/$ s].
X	spatial co-ordinate in the biofilm [m].
X_b	biomass concentration in biofilm [g/m^3].
Z	axial co-ordinate [m].
RE	removal efficiency.
C_{gin}	logarithmic average of the inlet concentrations of pollutants.
C_{gout}	logarithmic average of the outlet concentrations of pollutants.
EC	elimination capacity [g/m^3 h].
EC_{max}	maximum elimination capacity [g/m^3 h].
δ	biofilm thickness [m].
ε	bed porosity.
X_b	biomass density in biofilm.
X_r	biomass density in reactor.
u_g	surface velocity [m/s].
L	mass loading rate [g/m^3 h].
r_s	Acrylonitrile degradation rate [g/m^3 h].
V_f	bio-filter volume [m^3].
H	Henry's coefficient [$atm.mol^{-1}m^3$].
D	gas dispersion coefficient [m^2/s].

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