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A Mathematical Model for Removal of VOC's From Polluted air Utilizing a Biofilter

Leila Vafajoo*, Ali Naserranjbar, Farhad Khorasheh

Department of Chemical and Environmental Engineering, Islamic Azad University, Tehran South Branch, Tehran, Iran
vafajoo@azad.ac.ir

Recently, for the elimination or reduction of volatile organic compounds (VOC's) biofilters are being utilized more often. Degradation of the VOC's is made possible upon different packing of immobilized microbes. When removing such compounds as toluene in waste gases through a biofilter, clogging phenomenon will occur over time due to the formation of excessive biomass accumulation on the packing hence increasing of biofilm thickness. This phenomenon causes changes in the bed porosity and a subsequent increase in pressure drop and flow channelling which will eventually reduce the efficiency of the biofilter. In This study, differential equations related to the concentration distribution of toluene in the gas phase, Mass balance in the biofilm and the growth of microorganisms in a biofilter packed with spherical particles made of silica walls (R-635 Celite) with an equivalent diameter of 6mm were developed while simultaneously and dynamically solved with the MATLAB software. Consequently, the dynamic behavior of biofilter was predicted. Inlet gas stream contained 0.5 mg/l toluene in air and biofilm thickness and bed porosity of the biofilter at the start of operations, were 10^{-6} m and 34 %; respectively. These parameters changed to $350*10^{-6}$ m and 6 %; respectively after 92 hours. The toluene conversion also reached 82 % at this time. In order to ensure accurate modeling, the results of the mathematical model were compared with the existing experimental data of a biofilter and 14 % error was calculated. It seems that the error is due to physical properties of fluid assumed to be constant during the operation. However, the mathematical modeling in this area is very scarce and most researches on biofilter were experimental.

1. Introduction

Since the enactment of the 1990 Amendments to the Clean Air Act (CAA), technologies including adsorption, absorption, condensation, incineration, flaring, and biological control methods have been developed for the removal of VOCs and odors from waste gases (Yang et al., 2010). Many volatile organic compounds (VOCs) are classified as hazardous air pollutants (HAPs), and have been emitted from various industrial complexes (Qi and Moe, 2006). Although, gas biofiltration is considered to be a cost effective and reliable technology for control of low-concentration waste gases contaminated by VOCs and other odors (Devinny et al., 1999).
Since pollutant degradation occurs at normal temperature and pressure, biofiltration represents a potentially energy-efficient and low-capital technology when compared to more energy demanding or capital intensive physical and chemical abatement processes, such as catalytic wet oxidation, incineration, scrubbing or regenerative adsorption. It is particularly cheap and reliable for treating off-gas streams having large flow rates at minute contaminant levels (Iliuta and Larachi, 2004b). It has also become known as an environmental friendly technology due to environmentally benign end-products of

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water and carbon dioxide (Alonso et al., 1998). The Achilles' heel biofilters recognized to suffer from in waste gas treatment is the bed clogging induced by excessive microbial biomass accumulation (Cox and Deshusses, 1999). Excess biomass formation in a biofilter induces progressive clogging of the medium bed and a consequent buildup in pressure drop and flow channeling within this bed (Iliuta and Larachi, 2004a).

Due to the important role of production and accumulation of biomass in biofilteration, its prediction with help of simulation considered to be significant. Modeling facilitates a better understanding of the relationship between parameters and the removal of pollutants in order to predict biofilter performance. Furthermore, it makes it possible to optimize the biological process. In this study, a mathematical model to predict the dynamic behavior of a biofilter used for the biodegradation of toluene with nitrate as nitrogen source with the following stoichiometry is developed:

$$C_7H_8 + 6.29O_2 + 0.39NO^{-3} + 0.39H^+ \rightarrow 0.39C_5H_7O_2N + 2.8H_2O + 5.06CO_2 \quad (1)$$

2. Mathematical modeling of biofilter

To investigate effects of parameters in a biofilter on its performance, a mathematical model was developed. In the model differential equations of concentration distribution along the bed length, mass balance in the biofilm, biofilm thickness variations, the growth of microorganisms and the variation of bed porosity were all studied through solving the related equations simultaneously. Hence, the behavior of biofilter was investigated. In this study the physical characteristics of the modeled biofilter were based on values provided in Table 1.

Table 1: Biofilter characteristics used in this research

Parameter	Value	Unit
Pressure	1	atm
Reactor diameter	0.146	M
Bed height	1.12	M
Equivalent diameter of support particle	0.006	M
External porosity	0.34	-
Superficial gas velocity	0.05	m/s
Dry cell mass/wet cell volume	670,000	mg/L
Total dry biomass in the biofilm/wet	17,000	mg/L
Initial biofilm thickness	10-6	M
Distribution coefficient	0.27	ppmv/(mg/L)
sphericity factor	0.857	-

A unidirectional and single phase air flow containing toluene enters the porous bed and diffusion in biofilm begins. Toluene biodegradation by the microbes immobilized on 6 mm R-635 Celite considered for this purpose. It is reiterated that, immobilized microbes on these particles which are in the biofilm layer were responsible for degradation of toluene. In addition, assuming laminar flow in the gas and no reaction in this phase moreover; neglecting the axial direction diffusion, the equation of concentration distribution along the bed became as follows:

$$\frac{\partial}{\partial t}(C_{Sg}\varepsilon) + u_g \frac{\partial}{\partial z}(C_{Sg}\varepsilon) = D_g \frac{\partial^2}{\partial z^2}(C_{Sg}\varepsilon) - r_s a_s^0 \delta_b \eta \quad (2)$$

The initial and boundary conditions for solving equation (2) were provided as:

$$t = 0 \qquad C_{Sg} = C_{Sg}^{in} \quad (3)$$

$$z = 0 \qquad u_g C_{Sg}^{in} = u_g C_{Sg}\Big|_{z=0^+} - D_g \frac{\partial C_{Sg}}{\partial z} \quad (4)$$

$$z = H \qquad \frac{\partial C_{Sg}}{\partial z} = 0 \tag{5}$$

In addition, assuming solid particles in the biofilm growth will not be in contact with one another, the biofilm thickness will be estimated by the following equation (Alonso et al., 1997):

$$\frac{\partial \delta_b}{\partial t} = (r_d D_{S,w} \frac{\partial C_S}{\partial r}\Big|_{r=r_b}) \frac{Y_{X/S}}{\rho_v} - \delta_b b \tag{6}$$

Initial condition of equation (6) was:

$$t = 0 \qquad \delta_b = 10^{-6}\, m \tag{7}$$

Total shear/decay biomass are determined by b coefficient which is calculated as below (Alonso et al., 1997):

$$b = b_d + b_s \tag{8}$$

The specific decay coefficient was assumed to be constant (b_d) and the specific shear rate (b_s) was taken to be a function of biofilm thickness (Alonso et al., 1997):

$$b_s = b_{s0} (\frac{\varepsilon^0}{\varepsilon})^2 \tag{9}$$

Where b_{so} was the shear rate coefficient corresponding to the default shear stress when the bed was clean and no film was present. Through determining the amount of biofilm thickness at any time, the local porosity might have been calculated as (Iliuta and Larachi, 2004b):

$$\varepsilon = \varepsilon^0 - (\delta_b a_S^0) \tag{10}$$

Solution of the Eq. (2) ultimately; needed an appropriate understanding of the concentration profiles of toluene within bioparticles so as to calculate an overall effectiveness factor. Such concentration profiles were determined by toluene diffusion flux within bioparticle along with toluene consumption rate by the cells in the biofilm. Solving the equation (2) at biofilm scale required following assumptions:

- Homogeneous biofilm was wherein toluene diffuses according to Fick's law and is consumed by microorganisms.
- In order to describe the biological parameters, activity of a purified culture cell was considered.
- Except toluene the growth-limiting nutrient; all other nutrients were present in excess.
- Effects of outward diffusion of metabolic products were neglected.
- Toluene depletion due to adsorption in the biofilm and solid particles were neglected.
- Internal wetting of solids was complete, and species diffusion inside particles occurred in liquid phase.

For toluene biodegradation, a Monod type rate expression utilized to describe the culture growth kinetics (Alonso et al., 1997), i.e.;

$$\mu = \frac{\mu_{max} C_S}{K_S + C_S} \tag{11}$$

Kinetic parameters describing the growth of microbial cultures were presented in Table-2 (Alonso et al., 1997). According to the described assumptions, the mass balance equation for the biofilm phase expressed in spherical coordinates to account for the curvature, corresponding boundary and initial conditions:

$$\varepsilon_b \frac{\partial C_S}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 D_{S,b}^{eff} \frac{\partial C_S}{\partial r}) - \frac{\mu \rho_v}{Y_{X/S}} \tag{12}$$

The initial and boundary conditions for solving equation (12) were as follows:

$$r = r_p \qquad \frac{\partial C_S}{\partial r} = 0 \tag{13}$$

$$r = r_b \qquad C_S\Big|_{r=r_b} = \frac{C_{Sg}}{m} \tag{14}$$

$$t = 0 \qquad C_S(r,0) = C_S^{in} \tag{15}$$

Because the biofilm thickness increased with time, Eq. (12) was indeed a moving boundary problem. Porosity of biofilm and diffusivity of toluene within the biofilm was calculated using the correlation developed by Tang et al. (1987):

$$\varepsilon_b = 1 - \rho_v / \rho_c \tag{16}$$

$$\frac{D_{S,w}}{D_{S,b}^{eff}} - 1 = 15.549 \times 10^{-4} \, exp[-321.812(r_b - r_p)] \tag{17}$$

In which r_b and r_p are expressed in cm.

Table-2: Kinetic parameters of the present model

Kinetic parameter	Value	Unit
$Y_{X/S}$	0.84	mg biomass/mg toluene
μ_{max}	0.125	-
K_s	0.018	mg toluene / l
Decay rate coefficient, b_d	0.15	h^{-1}
Default shear rate coefficient,b_{s0}	$2.08*10^{-4}$	h^{-1}

3. Modeling results

The equations developed in this model were all solved simultaneously by means of MATLAB software and compared with experimental results available in the open literature (Alonso et al., 1997). At the inlet concentration 0.2 mg/l toluene and the empty bed residence time in the first 45 days was set equal to 2 minutes and between 45th and 82nd days it was set equal to 1 minute. In Figure 1 these results are presented in terms of conversion of toluene versus time. It is seen that, the results of the developed model are in good agreement with the experimental results. This emphasized the validity of the model's predictions. Moreover, this figure demonstrated that, in the early days of starting the operation conversion rate increased sharply however; it reached a plateau after some 30 days. The Strategy used in accumulated biomass removal was backwashed since by the 82nd day almost a stable conversion rate was achieved. Because the rate of toluene degradation and biomass accumulation variations in the absence of the biomass decay terms (b) is very significant, other results were evaluated under such terms' characteristic parameters.

The local porosity profiles and subsequently the biofilm thickness for the inlet toluene concentration amount of 0.5mg/l in three different levels of biofilter were compared with other modeling results (Iliuta and Larachi, 2004b) available in the open literature (Figures 2 and 3). As might be seen thru these figures, increase in accumulation resulted in exponentially filling up of the biofilter over time. In these figures biofilm thickness is considered to be 1μm at the beginning of the process. Through Figure-2, it is clear that the biomass along the bed length was not uniformly distributed and the variation of accumulation was considerably depended upon the axial location.

Through the above figures it is seen that the mass accumulation at the entrance (z/H = 0) of the bed had the highest rate which was due to the high cell growth rate in this area. However, this rate decreased toward the outlet of the biofilter which was probably due to the system encountered deficiency in nutrients. With increase in biofilm thickness at each level, gas pores are decreased and with reduction in the bed porosity, clogging of the biofilter occurred eventually.

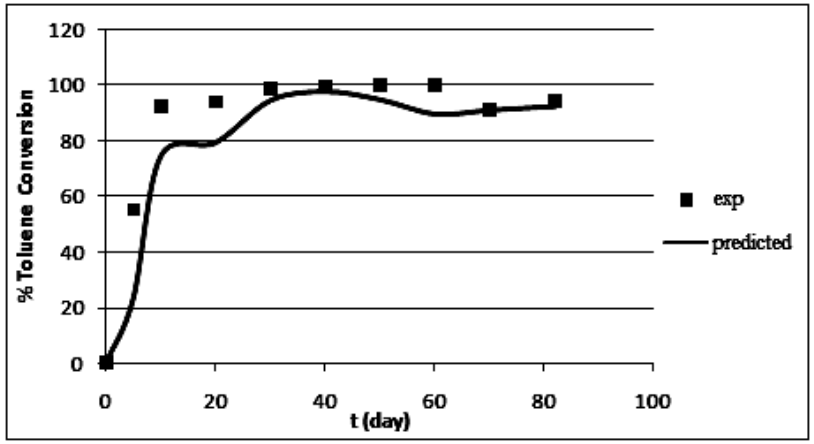

Figure 1: Variation of the conversion of toluene as a function of time for an 82 days period. Experimental results (■) are from Alonso et al. (1997).

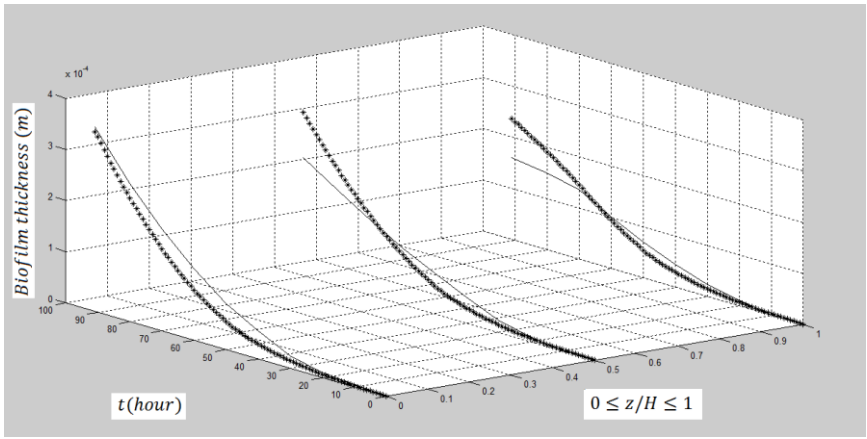

Figure 2: Variation in biofilm thickness versus time at three regions of the beginning, middle and end of the biofilter (solid lines are the mathematical results obtained through this study and dashed ones represent Iliuta and Larachi (2004b).

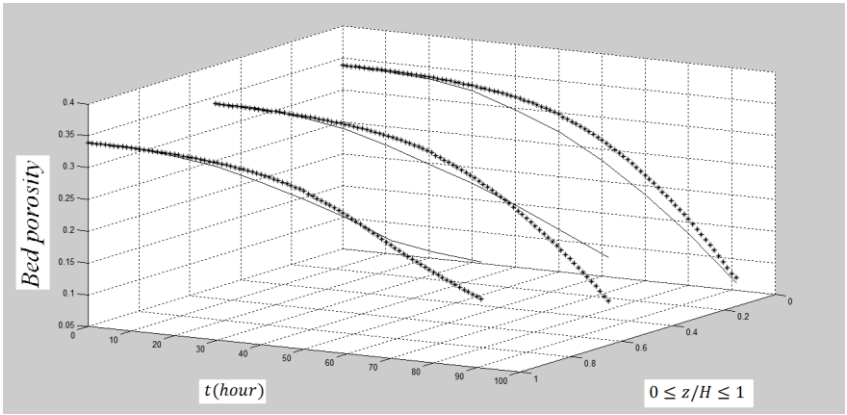

Figure 3: Variation of the bed porosity versus time at three different regions of the beginning, middle and end of the biofilter (solid lines are the mathematical results obtained through this study and dashed ones represent Iliuta and Larachi (2004b).

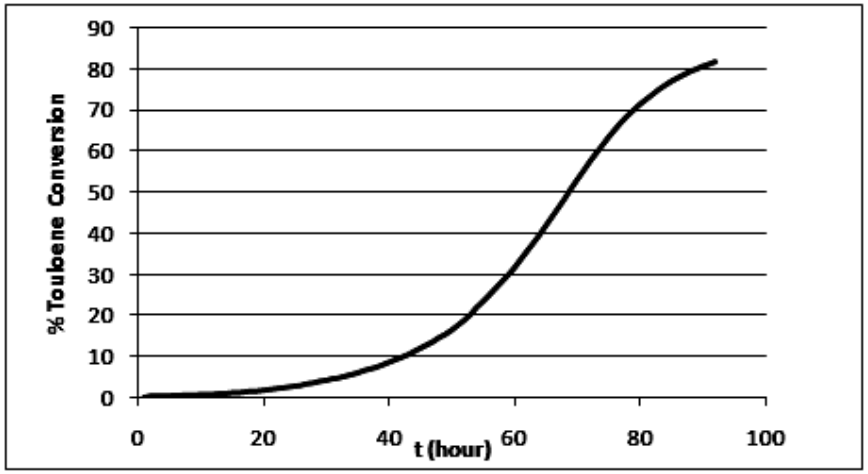

Figure-4: Conversion percentage of toluene during 92 hours

Figure 4 demonstrated the conversion of toluene during a 92 hours period for the system understudied. As it might be seen, the conversion of toluene was increased as time went by due to the enhancements of the biomass and subsequently the biofilm thickness. As soon as Biofilm thickness increased, the bed porosity decreased and therefore; by approaching to the end of the 92nd hour (*i.e.;* the end of profile), the slope of the curve was reduced.

4. Conclusion

In this study a one-dimensional dynamic mathematical model was developed based upon distribution of concentration in the gas phase, mass balance in biofilm and the growth of microorganisms in order to define the gas flow and the clogging period of time for the fixed bed biofilter. To begin with the decaying phenomenon was set equivalent to backwashing in real processes from which some theoretical results were determined. Comparison of these results with experimental data available in the open literature validated the model hence; led to predict the understudied system's behavior. In the next step without considering the decaying phenomenon, the time of biofilter clogging was predicted. The effect of biomass accumulation versus variation of bed porosity and biofilm thickness showed that the biomass accumulation at the beginning zone of the biofilter had the highest value due to the higher activity of microorganism in this region, over time however; this rate decreased towards the outlet of the biofilter. The formation of the additional biomass accelerated the occurrence of biofilter clogging. Ultimately, the conversion rate of toluene increased over time in a continuous manner from the beginning until the biofilter clogging where a plateau was reached. It is reiterated that the obtained results from this model are in good agreement with those of theoretical and experimental data determined by other researchers. This model paved down the road towards optimization of a rather complicated biological system.

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