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Numerical Solution and Sensitivity Analysis of Phenol Biodegradation

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Abstract:- In this study a mathematical model consisting of mass balance equation and accounting for reaction, mass transfer is developed to describe unsteady state phenol degradation in biofilter. For simulation purpose software BIOPHEN was developed in the language ForTran 77 and subsequently solved using Backward Implicit Scheme. The removal efficiency of phenol at inlet concentration is 99.47%. First order reaction kinetics is used .The concentration at different height and different time is obtained,which is not only useful for the design but is also applicable for predicting the concentration at various location and time of the bioreactor.The effect of parameter Specific surface area, biofilm thickness , and porosity on the performance of the biofilter were also investigated.

Key Words:- Biofilter, Modelling, Simulation, Reaction kinetics,Degradation

I. INTRODUCTION

Phenol is a common industrial chemical which is used in the manufacture of plastics, fibers, adhesives, iron, steel, aluminum, leather, and rubber. The presence of phenols in the environment is also related with production and degradation of pesticides and the generation of industrial and municipal sewages.[4]

Biofiltration is a new pollution control technology. It is an attractive technique for the elimination of low concentrations of volatile organic compounds (VOCs)([7]-[9]). Biofiltration treatment system are commonly applied to a wide range of volatile organic compounds where destruction of targeted compounds are achieved by passing through a porous support media onto which pollutant-degrading microorganisms are immobilized.([1],[13])

In this study a mathematical model consisting of mass balance equation describing unsteady state phenol removal along the length of a packed bed reactor is developed. The reactor is packed with a mixture of compost, perlite, sawdust and an activated sludge from paddy soil is taken for modelling purpose.To predict the concentration degradation of phenol in the biofilter,a model is required,which can be used for regulatory and planning purposes.Reliable model are needed to safeguard the public interest by contributing towards the monitoring of explosive gases in biofilter.The factors like porosity ,moisture content ,specific surface area,and effective diffusivity of gas in biofilm affecting the degradation of polluted gas in biofilter.

This study involves the development of a new technology that improve the air quality of the environment. Biofiltration is a cost effective technology utilizing natural and waste material that are available on site. The thrust of this work is to look at how fluctuating pollutant concentration in waste gases can be treated in biofilter, specifically biofilter performance in the removal of phenol. This work is relevant not only from an academic perspective but also from an industrial standpoint because it will advance engineering design and operation principles, which is key for commercial applications.

II. MATHEMAICAL MODEL

The mathematical model describing the biofiltration process is based on two main steps,diffusion of the phenol through the biofilm surrounding the packing material and its degradation in the biofilm in the presence of microorganisms([3],[5]-[6]).

For biological filter bed, it is supposed that the constituent particles are surrounded by a wet biofilm[10], as schematically illustrated in **Fig.1**. When air flows around the particles there is continuous mass transfer between the gas phase and the biofilm[11]. Phenol pollutants present in the waste gas, as well as oxygen, are partially dissolved in the liquid phase of the biofilm and are degraded or consumed by aerobic microbial activity.

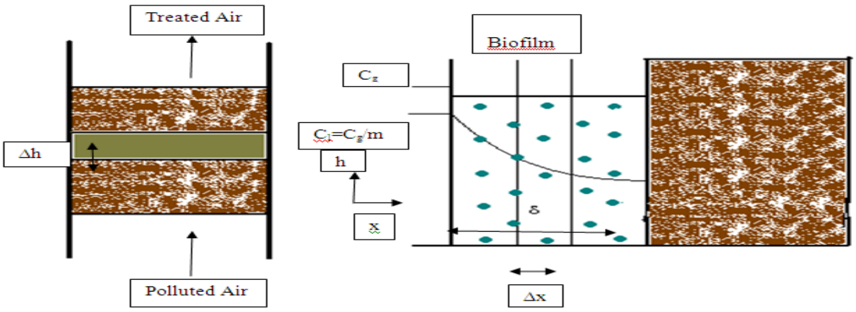

Fig:-1. Schematic Representation of the Model;h is the distance of the biofilter,x is the distance into the biofilm. δ is the biofilm thickness

The unsteady state model is based on the following assumptions.

(1) The biofilter is a porous and homogeneous body and biofilter assumed to behave as a bioreactor.
(2) The biofilm is formed on the exterior surface of the particles. Sizes of these pores are too small for microbial growth .[7]
(3) The biofilm is not necessarily formed uniformly around particles.
(4) Adsorption of the pollutant on the solid particles occurs only through the direct bare solid/air interface. Adsorption does not occur on the biofilm.
(5) Oxygen is not adsorbed on the solid particles since concentration gradient of oxygen between the gas phase and the solid is almost negligible.
(6) The extent of the biofilm patch is much larger than its depth.
(7) The phenol and oxygen at the biofilm and air interface are always in equilibrium as dictated by Henry's law.
(8) The phenol and/or oxygen are depleted in a fraction of the actual biofilm. This fraction is called the effective biolayer or active biofilm thickness ([9],[13])
(9) Diffusivities of the phenol is equal to the diffusivities of the same compounds in water, corrected by a factor depending on the biofilm density, according to the expression of [5]
(10) The biofilm density is constant.
(11) There is no accumulation of biomass in the filter bed and thus, the specific biofilm surface area is constant.
(12) The biodegradation rate depends on the concentration of the biofilm and oxygen.
(13) Direction of flow of phenol in vertical upward.
(14) Reaction in the bed is first order irreversible type.
(15) No axial dispersion[13]

These assumptions result in the following set of equations.

A mass balance of C_6H_6O in the bulk gas phase

$$\varepsilon \frac{\partial C_{C_6H_6O}}{\partial t} + Vg \frac{\partial C_{C_6H_6O}}{\partial h} = A_S D_e \left(\frac{\partial C_l}{\partial x} \right)_{x=0} \tag{1}$$

A mass balance of C_6H_6O in the biofilm

$$\frac{\partial C_l}{\partial t} = D_e \left(\frac{\partial^2 C_l}{\partial x^2} \right) - (-r_{C_6H_6O}) \tag{2}$$

Microkinetics

Microkinetics is characterized by first order rate of reaction. Thus the reaction rate for C_6H_6O is given by

$$(-r_{C_6H_6O}) = k_1 C_l \tag{3}$$

Where, $(-r_{C_6H_6O})$ is degradation rate of C_6H_6O, gm m^{-3} h^{-1}

k is rate constant , h^{-1},C_l is concentration in the biofilm (g/m^3), equation (2) becomes

$$\frac{\partial C_l}{\partial t} = D_e\left(\frac{\partial^2 C_l}{\partial x^2}\right) - k_1 C_l \tag{4}$$

Assuming dynamic equilibrium between the gas phase and the surface of the biofilm, a pseudo-steady state assumption is made for the biofilm and accumulation term is set to 0. in Equation (4)

$$D_e\left(\frac{\partial^2 C_l}{\partial x^2}\right) - k_1 C_l \tag{5}$$

Boundry conditions

B.C. 1

For $t > 0$, $x = 0$, $C_l = \dfrac{C_{C_6H_6O}}{H_c}$

B.C. 2

At $t > 0$, $x = \delta$, $\dfrac{dC_l}{dx} = 0$

Where H_c is Henry's constant

Solution can be obtained as equation (5)

$$\left(\frac{\partial C_l}{\partial x}\right)_{x=0} = -m\frac{C_{C_6H_6O}}{H_c}\tanh(m\delta) \tag{6}$$

Where $m = \sqrt{\dfrac{k_1}{D_e}}$

Put equation (6) in equation (1) ,the final equation is

$$\varepsilon\frac{\partial C_{C_6H_6O}}{\partial t} + Vg\frac{\partial C_{C_6H_6O}}{\partial h} = -\varphi \bullet C_{C_6H_6O} \tag{7}$$

Where, $\varphi = \dfrac{A_S D_e m}{H_c}\tanh(m\delta)$

Initial and Boundary Conditions

IC

At $t = 0$, $h = 0$, $C_{C_6H_6O} = C_0$

For $t = 0$, $0 < h \le H$, $C_{C_6H_6O} = 0$ (8)

BC

At $t > 0$, $h = H$, $\dfrac{\partial C_{C_6H_6O}}{\partial h} = 0$

A. **Parameters**

All parameters are taken from published results.The values of the parameters used to solve the model equation are listed in table 1

Table.I

Variables	**Parameters**	**Units**	**Value**
$\mathbf{A_S}$	Specific surface area	$m^2\ m^{-3}$	413
He	Henry's Constant	-	0.42
$\mathbf{D_e}$	Effective Diffusivity	$m^2\ h^{-1}$	15.48×10^{-5}
$\mathbf{k_1}$	First order Rate Constant	h^{-1}	$0.35h^{-1}$
ε	Porosity	-	0.50
H	Height of Biofilter	m	0.4
δ	Biofilm Thickness	m	0.0003
∆h	Differential length along the column	m	0.04
∆t	Differential time element	h	15

III. NUMERICAL SCHEME

The model equation were solved using a computer code is developed in FORTRAN 77.The system of differential equation was solved by Backward Implicit scheme. This involve Descretization of the equation with respect to height and time. The reactor column height and time were descretized over a uniform grid. The grid is result in a tridiagonal matrix of the solution. The equation in matrix form is

$$A \times C = P \quad (9)$$

C is the solution vector .The value of C is obtained based on a method developed(Srivastava,1983).

IV. RESULTS AND DISCUSSION

The simulated results are presented here in the form of graph.

A. Phenol concentration In The Biofilter With The Increase In Height And Time

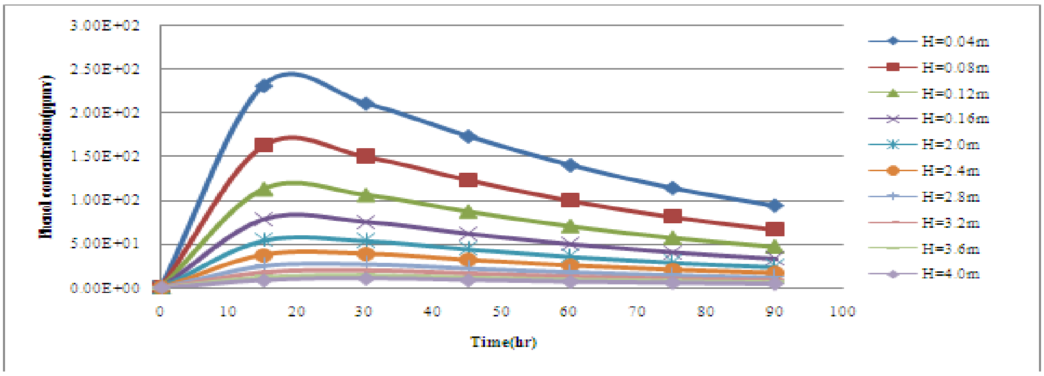

Fig.2. Phenol concentration Vs Time at Various Height
C_0=891ppmv,As=413m^2/m^3,De=15.48×$10^{-5}m^2/h$,δ=0.0003m,k_1=0.35h^{-1},Q=0.0125m^3/h,ε=0.50

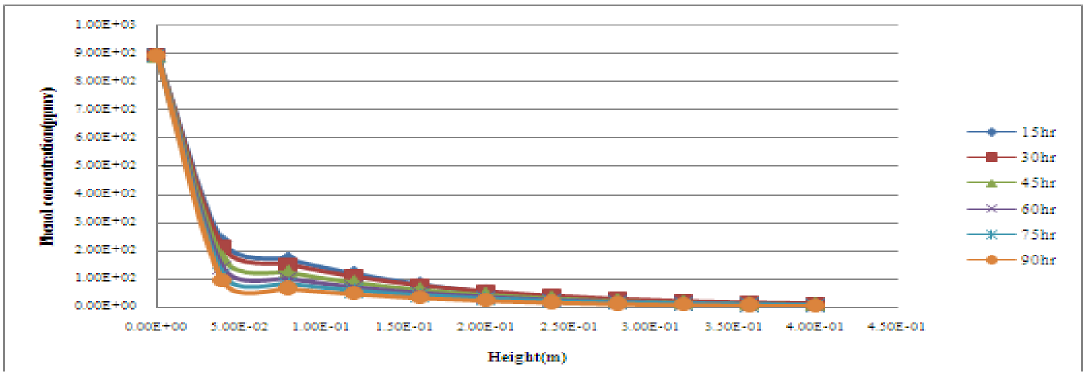

Fig.3. Phenol concentration Vs Height at Various Time
C_0=891ppmv,As=413m^2/m^3,De=15.48×$10^{-5}m^2/h$,δ=0.0003m,k_1=0.35h^{-1},Q=0.0125m^3/h,ε=0.5

Fig 2 shows the variation of phenol concentration with respect to time in the biofilter height.It is observed that phenol concentration decrease with the increase in height.This is due to fact that as bed height increases as a result of which capacity of biofilter increases resulting in the decreased outlet phenol concentration. And Fig 3. shows the variation of phenol concentration with respect to height in the biofilter with varying time.This is due to the reason that with the elapse of time microbe's population grows there by more and more phenol concentration is consumed.

B. Simulated Result For Heigher Efficiency

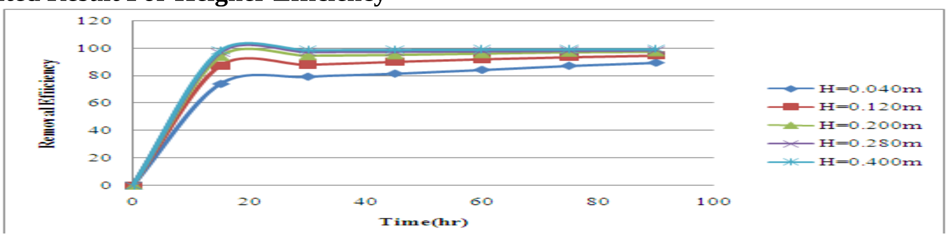

Fig.4. Removal efficiency Vs Time at various Heights
C_0=891ppmv, As=413m^2/m^3,De=15.48×$10^{-5}m^2/h$,δ=0.0003m,k_1=0.35h^{-1},Q=0.0125m^3/h,ε=0.50

Fig 4. shows the effect of the biofilter bed height increase in height on the efficiency. The removal efficiency obtained at 90 hr of phenol was 99.47%.Therefore the removal efficiency was increase with increase in the bed height.

C. Effect Of Specific Surface Area Of Biofilter Media On Phenol Concentration In Biofilter With Increasing Height And Time

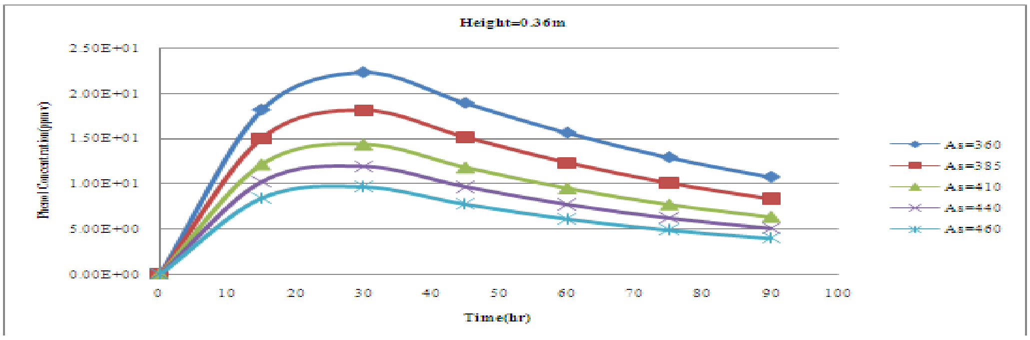

Fig.5. Phenol concentration Vs Time at Various As (Specific surface Area)
C_0=891ppmv,D_e=15.48×$10^{-5}$$m^2$/h,δ=0.0003m,$k_1$=0.35$h^{-1}$,Q=0.0125$m^3$/h,ε=0.50

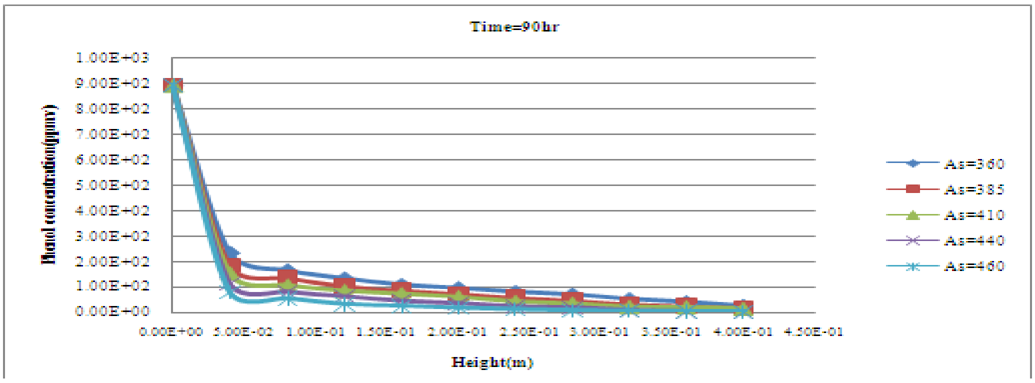

Fig.6. Phenol concentration Vs Height at Various As (Specific surface Area)
C_0=891ppmv,D_e=15.48×$10^{-5}$$m^2$/h,δ=0.0003m,$k_1$=0.35$h^{-1}$,Q=0.0125$m^3$/h,ε=0

Fig 5 Shows the effect of specific surface area of biofilter media on phenol concentration in the biofilter with respect to time. The effect of the specific surface area on the exit gas concentration, the outlet phenol concentration was found to be decreasing with the increase in specific surface area. From this ,it is evident that with higher specific surface area the removal is increased. This is intuitively expected because for a given biofilm thickness increased surface area increases the reaction volume and area of mass transfer. And Fig 6 shows the effect of specific surface area of biofilter media on phenol concentration in the biofilter with respect to height. The outlet phenol concentration is found to be decreasing with the increase in specific surface area this is due to fact that with increase in surface area more and more phenol is consumed .Therefore there is a decrease in the outlet phenol concentration.

D. Effect Of Porosity On Phenol Concentration In Biofilter With Increasing Height And Time

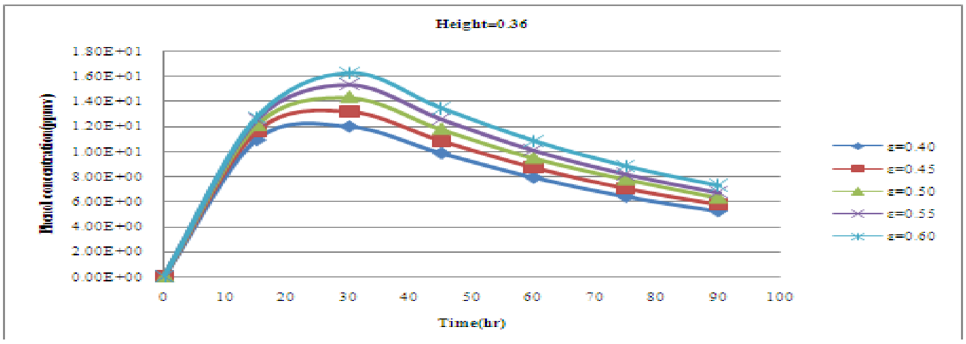

Fig.7. Phenol concentration VsTime at Various ε(Porosity)
C_0=891ppmv,A_S=413m^2/m^3, k_1=0.35h^{-1}, D_e=15.48×$10^{-5}$$m^2$/h ,δ=0.0003m ,Q=0.0125$m^3$/h

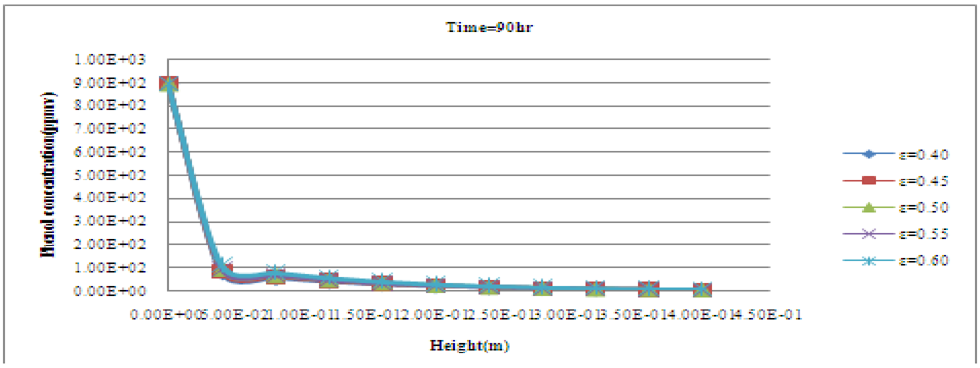

Fig.8. Phenol concentration Vs Height at Various ε(Porosity)
C_0=891ppmv,A_S=413m^2/m^3, k_1=0.35h^{-1}, D_e=15.48×$10^{-5}$$m^2$/h ,δ=0.0003m ,Q=0.0125$m^3$/h

Fig 7. shows that shows the effect of porosity of the biofilter media on phenol concentration in the biofilter with respect to time..The phenol concentration is found to be increasing with the increase in porosity .This is due to fact that with the increase in porosity ,the biofilter media available for the degradation decreases, hence there is an increase in the phenol concentration .Fig 8. shows the effect of porosity of the biofilter media on phenol concentration in the biofilter with respect to time. The phenol concentration is found to be increasing with the increase in porosity.

E. Effect of Biofilm Thickness on Phenol Concentration In Biofilter With Increasing Height And Time.

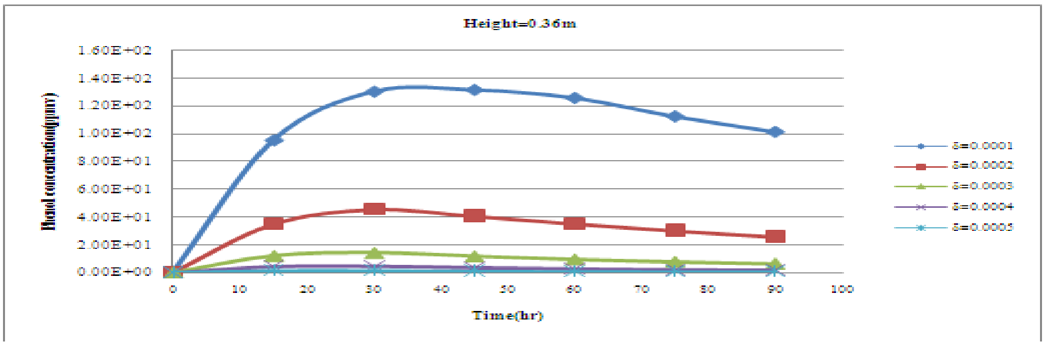

Fig.9. Phenol concentration Vs Time at Various δ(Biofilm Thickness)
C_0=891ppmv,A_S=413m^2/m^3, D_e=15.48×$10^{-5}$$m^2$/h, k_1=0.35h^{-1}, Q=0.0125m^3/h,ε=0.50

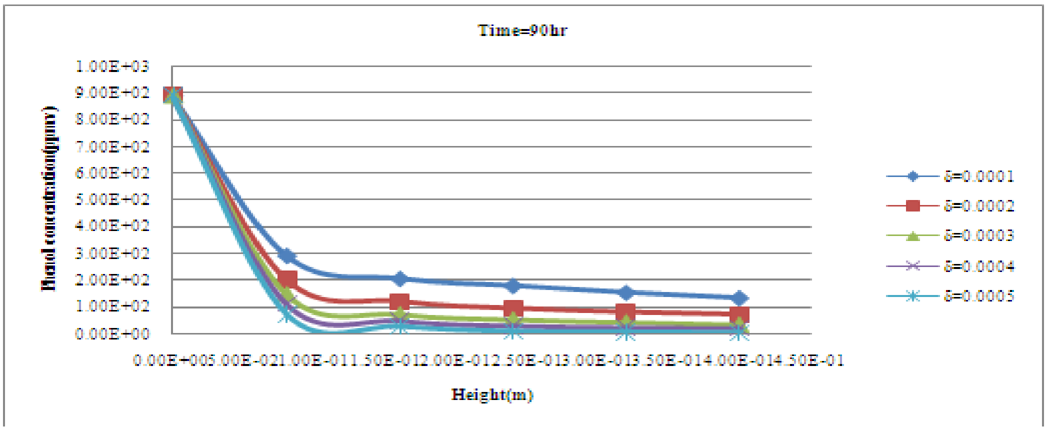

Fig.10. Phenol concentration Vs Height at Various δ(Biofilm Thickness)
C0=891ppmv,AS=413m2/m3, De=15.48×10-5m2/h, k1=0.35h-1, Q=0.0125m3/h,ε=0.5

Fig 9. shows the effect of biofilm thickness on phenol concentration in the biofilter with respect to time..The phenol concentration was found to decrease with the increase in the thickness of biofilm. This is due to the fact that with the increase in biofilm thickness more and more phenol concentration is consumed as a result of reactions, resulting in the decrease of the outlet phenol concentration from the biofilter.And Fig10. shows effect of the biofilm thickness on phenol concentration in the biofilter with respect to height. The phenol concentration is found to decrease with the increase the biofilm thickness .Because of the increase in the thickness higher concentration of phenol used up as the depth is increased and decreasing the net outlet phenol concentration.

IV. CONCLUSIONS

In this work the results shows that the phenol concentration was decrease with the increase in height and time. It was also observed that with increasing time and height the outlet phenol concentration is found to decrease with the increase in the value of parameters namely specific surface area and biofilm thickness. and with increase time and height the outlet phenol concentration increase with the increase in the value of parameter porosity. Simulated maximum phenol removal efficiency is observed to be 99.94%.

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