Modeling of fungal biofilter for the abatement of hydrophobic VOCs

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ABSTRACT

This work describes the growth of filamentous fungi in biofilters for the degradation of hydrophobic VOCs. The study system was n-hexane and the fungus *Fusarium solani* B1. The system is mathematically described and the main physical, kinetic data and morphological parameters of aerial hyphae were obtained by independent experiments for model validation. The model proposed in this study describes the increase in the transport area by the growth of the filamentous cylindrical mycelia and its relation with n-hexane elimination in quasi -stationary state in a biofilter. The model describing fungal growth includes Monod-Haldane kinetic and hyphal elongation and ramification. The reduction in the permeability caused by mycelial growth was further related to pressure drop by Darcy's equation. The model was verified with biofiltration experiments using perlite as support and gaseous n-hexane as substrate.

1 INTRODUCTION

Biofiltration is one of the main techniques for the control of volatile organic compounds (VOCs) present in low concentrations in industrial gaseous emissions. The high flow-rate of such emissions means that the investment and operating costs for conventional systems are high. In these systems, microorganisms fixed in a solid support oxidise the VOCs, principally to CO_2 and water.

Due to the complexity of the system, resulting from its inherent heterogeneity and the diversity of the microbial populations which may become established, biofilters are difficult to model. The modelling of these systems involves physical and biochemical steps, liquid flow and diffusion, the properties of the microbial community and the solid support, prediction of the area and active thickness of the biofilm, etc (Bibeau *et al*., 2000). One of the main considerations when modelling biofilters is the assumption that the biomass and the liquid film which surrounds it form a single pseudo-homogeneous phase known as the biofilm.

Ottengraf and van der Oever (1983) developed a solution to analyse the concentration profile in the biofilm and throughout the biofilter column to obtain the quantity of contaminant biodegraded in the biofilter, using first order and order zero growth kinetics.

Shareefdeen and Baltzis (1994) developed a model for a fixed bed biofilter with transitory state operation for the treatment of toluene, implementing mass balances in the biofilm, the gas phase and the solid support, and using a Monod microbial growth kinetic. Hodge and Devinny (1995) and Jorio *et al*. (2003) developed a model using four different types of support material, to describe the mass transfer between the air phase and solid/water, the biodegradation of the substrate, CO_2 production and changes in the pH as a result of CO_2 accumulation. They also assumed that the filter medium and the distribution and density of the biomass in the biofilm is homogeneous and that the adsorption is reversible. The same assumptions are made by Deshusses *et al*. (1995), using a Monod type growth kinetic, with competitive inhibition for a mixture of methyl isobutyl ketone and methyl ethyl ketone.

The mathematical model to describe the biofiltration of mixtures of hydrophilic and hydrophobic compounds used by Mohseni and Allen (2000) is based on the biophysical model proposed by Ottengraf and van den Oever (1983) for a VOC. The steady state model was developed considering the biofilm as an organic matrix and using Monod growth kinetics with inhibition.

Iliuta and Laranchi (2004) describe the growth of the biofilm and its effect on the aerodynamics and clogging of the biofilter. The model considers a uni-directional flow based on the volumetric average of the balance of mass, momentum and species, linked to the conventional equations for diffusion/reaction in biological systems.

Spigno *et al*. (2003) made a simple, steady state, axial dispersion model to evaluate the n-hexane elimination in a biofilter using the fungus *Aspergillus niger*. This model makes the same assumptions as those used for microbial consortia or bacterial biofilters, working with a constant, homogeneous fungus biofilm. The balance in the biological phase included a Monod type biodegradation with substrate inhibition.

In general, it may be observed that the models which have been developed are based on the structure of a biofilm as a pseudo-homogeneous phase. However in the case of aerial biofilms, as those generated by filamentous fungi, this definition is not

readily applicable. Although good results are obtained, they do not provide good information on the actual phenomena occurring in the inter-particular spaces of the biofilter and the growth characteristics of the fungus inside the biofilter. The objective of this work is to describe the growth of the filamentous fungi on a biofilters for the degradation of hydrophobic VOCs. The study system was n-hexane, as a model substrate and the fungus *Fusarium solani* B1.

2 MATHEMATICAL MODEL

2.1 Definition of the system

The model proposed in this study describes the increase in the transport area by the growth of the filamentous cylindrical mycelia and its relation with n-hexane elimination in quasi -stationary state in a biofilter. To mathematically describe the system, we considered four processes: (1) mass transfer of VOCs in the bulk gas, (2) mass transfer of VOCs into the gas layer around the mycelium, (3) mass transfer and reaction of the nitrogen source through the elongating mycelia, (4) and the kinetic of mycelial growth. Processes (2) and (3) include movable boundary conditions to account for the mycelial growth. The model describing fungal growth includes Monod-Haldane kinetic (Shuler *et al*., 2003) and their elongation and ramification and is further related to macroscopic parameters such as pressure drop. The basic concept of the model develop was obtained using the Figure 1.

2.2 Mechanism of growth

The biomass and total length were determinate considering the principal hyphae and the branching.

$$\frac{dL_h}{dt} = (\mu L_{AV})\left(1 - \frac{\beta L_h}{L_{max,m}}\right) + (\varphi L_h)\left(N_{TB} - \frac{\gamma\beta L_h}{L_{max,B}}\right) \tag{1}$$

2.3 Mass balance in the biofilter

Unidirectional gas flow was considered:

$$\frac{\partial \mathcal{C}_{Ab}}{\partial Z} - \frac{1}{Pe_l}\left(\frac{\partial^2 \mathcal{C}_{Ab}}{\partial Z^2}\right) = S_t\left(\mathcal{C}_{Ab} - \mathcal{C}_{AG}\right) \tag{2}$$

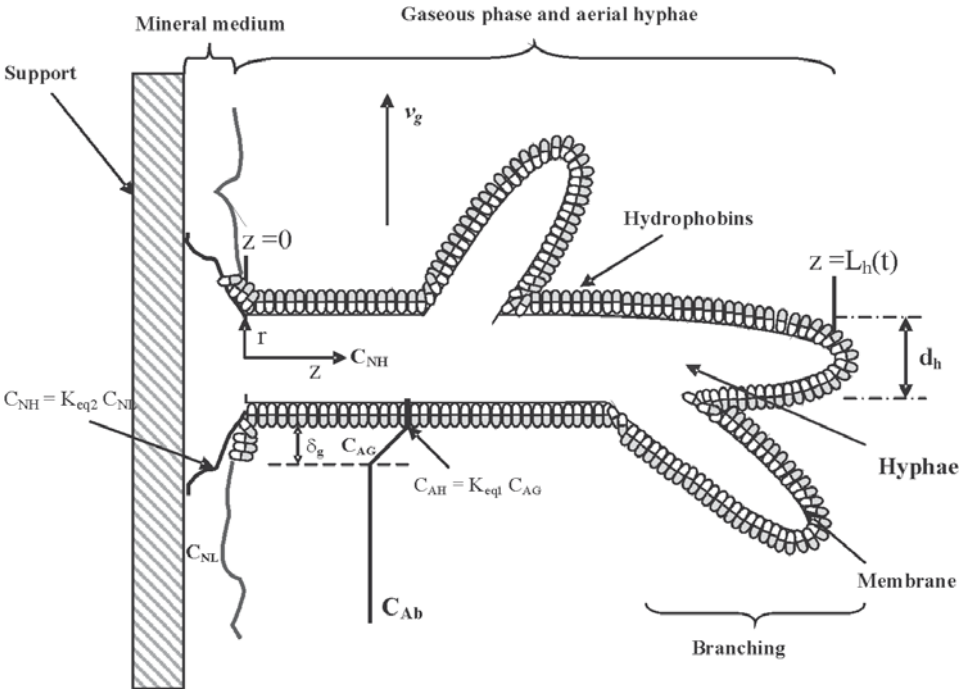

Figure 1. Schematic representation of growth.

Axial boundary condition that consider the continuity of flux to the right of z = 0 and z = H (Illiuta and Larachi, 2004).

$$\text{C.F.1} \quad Z = 0 \quad \left.\mathscr{C}_{Ab}\right|_{Z} = \left.\mathscr{C}_{Ab}\right|_{Z+\Delta Z} - \frac{1}{\mathrm{Pe}_1}\left.\frac{\partial \mathscr{C}_{Ab}}{\partial Z}\right|_{Z+\Delta Z} \tag{3}$$

$$\text{C.F.2} \quad Z = 1 \quad \frac{\partial \mathscr{C}_{Ab}}{\partial Z} = 0 \tag{4}$$

Where: $\mathscr{C}_{Ab} = \dfrac{C_{Ab}}{C_{Abo}}$; $Z = \dfrac{z}{H}$; $\mathscr{C}_{AG} = \dfrac{C_{AG}}{C_{Abo}}$; $\mathrm{Pe}_l = \dfrac{Hv_g}{D_{Dz}}$; $S_t = \dfrac{k_g a_v H}{v_g}$

To determine the flow regime around the hyphae, the criterion reported by Slattery (1999) was used and found that it can be considered *creeping flow* (*Reynolds* number around hyphae of 0.002).

$$\cos\theta\left[1+\frac{1}{\xi^2}\right]\frac{\partial \mathscr{C}_{AG}}{\partial\xi}+\frac{\text{sen}\theta}{\xi}\left[\frac{1}{\xi^2}-1\right]\frac{\partial \mathscr{C}_{AG}}{\partial\theta}=\frac{1}{\text{Pe}_2}\left[\frac{1}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial \mathscr{C}_{AG}}{\partial\xi}\right)\right] \tag{5}$$

The boundary conditions incorporate the interaction in the gas-hyphae interphase.

C.F.1. $\xi=\delta_G \qquad \mathscr{C}_{AG}=\dfrac{C_{Ab}}{C_{Abo}}$ (6)

C.F.2. $\xi=1 \qquad -\dfrac{\partial \mathscr{C}_{AG}}{\partial\xi}=\left[w_1\times\left(\dfrac{\mathscr{C}_{AG}}{\mathscr{C}_{AG}+K_1+\dfrac{\mathscr{C}_{AG}^2}{K_I^*}}\right)\left(\dfrac{\mathscr{C}_{NH}}{\mathscr{C}_{NH}+K_2}\right)+w_2\right]\times\lambda(t)$ (7)

C.F.3. $\theta=0 \qquad \mathscr{C}_{AG}=\dfrac{C_{AG}}{C_{Abo}}$ (8)

C.F.4. $\theta=\dfrac{\pi}{2} \qquad \mathscr{C}_{AG}=\dfrac{C_{AG}}{C_{Abo}}$ (9)

Where: $\mathscr{C}_{AG}=\dfrac{C_{AG}}{C_{Ab_O}}$; $\xi=\dfrac{r}{r_l}$; $\lambda(t)=\dfrac{L_h(t)}{2r_l}$; $\text{Pe}=\dfrac{r_l v_g}{D_g}$; $w_1=\dfrac{\mu_{max}}{Y_A}\times\dfrac{\rho_h\,4\pi r_l^3}{\delta_h D_g\,C_{Abo}}$;

$w_1=m_C\times\dfrac{\rho_h 4\pi r_l^3}{\delta_h\,D_g\,C_{Abo}}$; $K_1=\dfrac{K_{AH}}{C_{Abo}\,K_{eq1}}$; $K_2=\dfrac{K_{NH}}{C_{NLo}\,K_{eq2}}$; $\dfrac{1}{K_I^*}=\dfrac{K_{eq1}C_{Abo}}{K_I}$

In the development of the mass balance of the nitrogen source, diffusion and reaction throughout hyphae were considered.

$$\frac{\partial \mathscr{C}_{NH}}{\partial\tau}=\frac{\partial^2 \mathscr{C}_{NH}}{\partial Z_1^2}-\Phi^2\left[\frac{\mathscr{C}_{AG}}{\mathscr{C}_{AG}+K_1+\dfrac{\mathscr{C}_{AG}^2}{K_I^*}}\right]\left[\frac{\mathscr{C}_{NH}}{1+\mathscr{C}_{NH}\beta}\right] \tag{10}$$

The boundary condition and the initial condition for this equation are:

$$\text{C.I} \quad t = 0 \qquad C_{NH} = C_{NH_0} \tag{11}$$

$$\text{C.F.1.} \quad Z_1 = 0 \quad \mathcal{C}_{NH} = C_{NL} / C_{NL,o} \tag{12}$$

$$\text{C.F.2.} \quad Z_1 = 1 \quad \frac{\partial \mathcal{C}_{NH}}{\partial Z_1} = 0 \tag{13}$$

$$\text{Donde: } \beta = \frac{1}{K_2};\ \Phi = L_h \sqrt{\frac{\mu_{max} \times \rho_h}{Y_N \times D_{NH} \times K_{NH}}};\ \mathcal{C}_{AG} = \frac{C_{AG}}{C_{Abo}};\ Z_1 = \frac{z_1}{d_h};\ \mathcal{C}_{NH} = \frac{C_{NH}}{C_{NHo}};$$

$$\tau = \frac{D_{NH}\, t}{d_h}$$

2.4 Effect of the growth on the pressure drop

The pressure drop was evaluated as a function of the reduction in the permeability caused by mycelial growth in the bioreactor and the Darcy´s equation.

3 MATERIALS AND METHODS

3.1 Microorganisms and inoculum

Fusarium sp. was isolated as described by Arriaga and Revah (2005a). Its preservation, cultivation conditions and spore production was similar to reported for García-Peña *et al*. (2001). The biofilter was inoculated with a mineral medium solution and 2×10^7 spores mL^{-1}.

3.2 Carbon sources and mineral medium

The carbon source used was n-hexane (Baker, 98.5%). The mineral medium for fungi maintenance and cultivation was reported previously by Arriaga and Revah (2005a).

3.3 Biofilter system

The gas-phase biofilter consisted of a 1 m cylindrical glass column with inner diameter of 0.07 m, incubated at 30(±3)°C. The biofilter was packed with 250 g of

perlite (bed void fraction of 68% and particle size of 3.4 – 4.8 mm) mixed with the mineral medium and the spore solution. Hexane-saturated air was mixed with moistened air and introduced at the top of the biofilter with a flow rate of 1.2 L min^{-1}, with a residence time of 1.3 min, to reach an inlet n-hexane load of 325 g m^{-3} h^{-1}.

3.4 Analytical methods

Hexane concentration in biofilter system were measured with FID-GC and CO_2 production by TCD-GC. The biomass in the perlite was measured as volatile solids with a thermogravimetric analyzer. Measurements were done in triplicate. The pressure drop was measured online by using pressure transducer with a data acquisition system online.

4 RESULTS AND DISCUSSION

4.1 Validation of the mathematical model

The Figure 2 and 3 shows the comparisons between the experimental results obtained in biofilter and model simulation. For the model simulation the data shown in Table 1 were used.

4.1.1 Elimination capacity (EC)

Figure 2 compares the experimental data and the mathematical model for different cellular yield coefficients. In biological systems, when growth is uncoupled with the energy metabolism, the constant cellular yield for growth does not represent the reality of biomass production. This can be one of the explanations of the greater EC observed in Figure 2 with respect to the model prediction for low values of cellular yield (0.1 $g^{-1}g^{-1}$) when the growth in the fungi starts, existing differences of 2% between the experimental data and the model. Similarly it is possible to explain the low EC obtained with the simulation during the latency stage, greater cellular yield coefficients (0.8 g^{-1} g^{-1}), existing differences of 12% between the experimental data and the model.

In general, it is possible to observe an average deviation between the model and the experimental data for the EC of 7%.

4.1.2 Pressure drop

The Figure 3 shows the comparison of the experimental results of the pressure drop (ΔP) in the biofilter and the model simulation. The Figure 3 shows that in the first days of operation, before obtaining an important biomass growth, the ΔP determined by the model was in average 11% lower than experimental data, presumably due to the static liquid present in the bed, necessary to maintain the humidity of the biofilter, which was not considered in the model. On the other hand, it is possible to

observe that for the ΔP simulated after 30 days operation was obtained an average deviation of the experimental data of 3%.

Table 1.
Parameters used in simulations.

Parameter	Value	Unit	Reference
Kinetic parameter			
K_{AH}	1.9	g m^{-3}	[1]
K_{NH}	500	g m^{-3}	[1]
K_I	30.1	g m^{-3}	[1]
m_C	1.51×10^{-4}	g g h^{-1}	[1]
μ_{max}	0.0518	h^{-1}	[1]
Y_N	2.546	g g^{-1}	[2]
Y_A	0.824	g g^{-1}	[2]
Morphological parameters			
λ	0.35	—-	[2]
γ	2.47	—-	[2]
d_h	2.10	μm	[2]
L_{av}	280.1	μm	[2]
$L_{max,m}$	1477	μm	[2]
$L_{max,B}$	452.1	μm	[2]
L_C	665.6	μm	[2]
L_o	8.34	μm	[2]
N_{TB}	7.0	—-	[2]
N_0	1.0×10^{4}	—-	[2]
ρ_h	1.1×10^{-9}	mg μm^{-3}	[3]
Physical-chemical parameters			
H	1.0	m	—-
$\varepsilon_{R\ (initial)}$	0.685	m^3 m^{-3}	—-
d_p	0.004	m	—-
D_g	0.029	m^2 h^{-1}	—-
v_g	48.91	m h^{-1}	—-
ρ_g	1160	g m^{-3}	[4]
μ_g	64.98	g m^{-1} h^{-1}	[4]
D_{NH}	5.7×10^{-6}	m^2 h^{-1}	—-
D_{Dz}	0.079	m^2 h^{-1}	—-
k_g	36.56	m h^{-1}	—-
HPC	0.20	—-	[1]

[1] Vergara-Fernández *et al*. (2006), [2] Vergara-Fernández, (2007), [3] López-Isunza *et al*. (1997), [4] Hartmans y Tramper (1991).

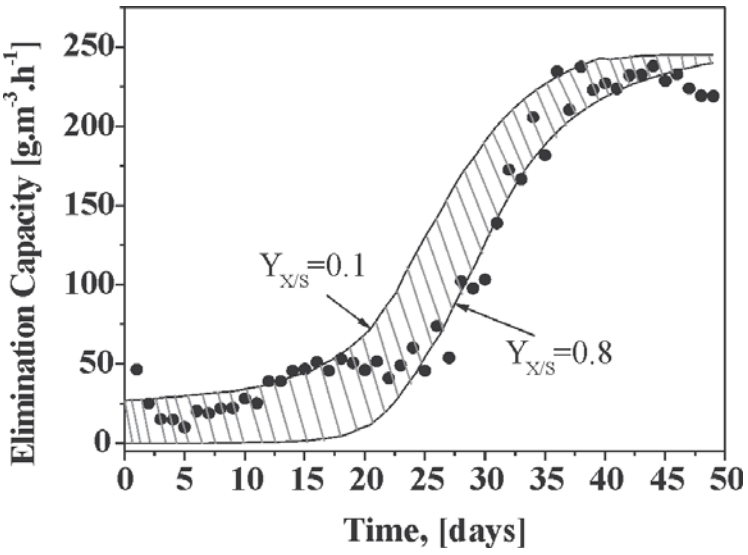

Figure 2. Experimental EC and model simulation. (•) Experimental results and (–) simulation. Variation of the EC simulation for a range of cellular yield in *F. solani* between 0.1 and 0.8 $g^{-1}g^{-1}$.

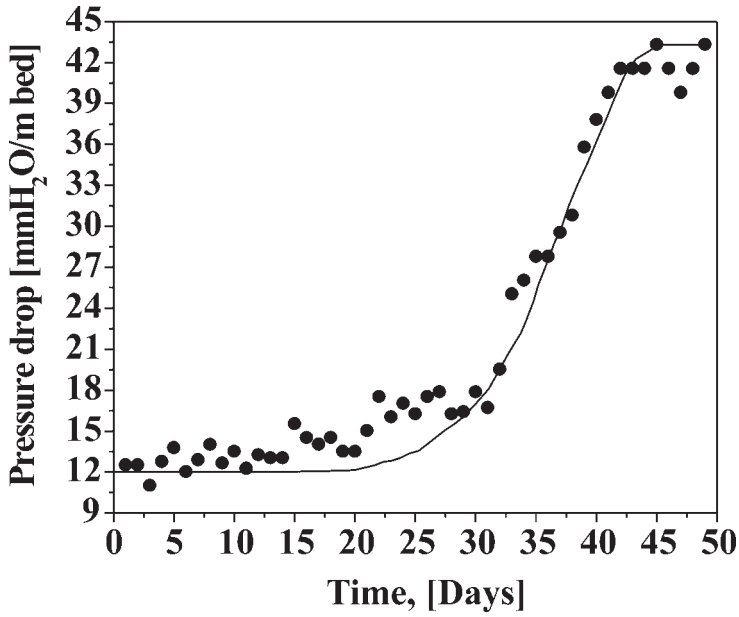

Figure 3. Experimental evolution of the pressure drop in the biofilter and model prediction. (•) Experimental data and (–) simulation.

5 CONCLUSIONS

Growth of fungi and n-hexane elimination was modeled in biofiltration systems connecting a growth model based on microscopic parameters and the different mass balances describing the main transport phenomena occurring inside a biofilter. The independent evaluation of the parameters allowed a small deviation with experimental data below 10% for the elimination capacity and the pressure drop.

6 NOMENCLATURE

a_v : Specific area, [L^2/L^3]
C_{Ab} : n-hexane concentration in the bulk, [M/L^3]
C_{AG} : n-hexane concentration in the gas film, [M/L^3]
C_{AH} : Extra-cellular COV concentration, [M/L^3]
C_{NH} : Nitrogen source concentration in the hyphae, [M/L^3]
C_{NL} : Nitrogen source concentration in liquid, [M/L^3]
d_h : Average diameter of the hyphae, [L]
D_{Dz} : Axial dispersión coefficient, [L^2/T]
D_g : n-hexane diffusivity, [L^2/T]
D_{NH} : Nitrogen source diffusivity in the hyphae, [L^2/T]
H : Biofilter height, [L]
k_g : Mass transfer coefficient of gas, [1/T]
K_{AH} : Affinity constant of n-hexane, [M/L^3]
K_{NH} : Affinity constant of nitrogen, [M/L^3]
K_I : Inhibition constant, [M/L^3]
K_{eq1} : Equilibrium constant of n-hexane/hyphae
K_{eq2} : Equilibrium constant of nitrogen source/hyphae
L_{av} : Average length of the hyphae, [L]
$L_{max,m}$: Average maximum distal length of the individual hyphae, [L]
$L_{max,B}$: Average maximum distal length of the branching, [L]
L_h : Individual total length of hyphae, [L]
$L_{h,Total}$: Total length of the hyphae, [L]
m_C : Cellular maintenance coefficient, [1/T]
N_{TB} : Branching number in individual hyphae
N_0 : Initial number spores
V_R : Reactor total volume, [L^3]
V_E : Total volume of the support, [L^3]
v_g : Average lineal rate of the gaseous phase, [L/T]
υ_g : Gas film rate, [L/T]

$X_{h,Total}$: Total biomass, [M]
Y_A : n-hexane cellular yield, [M/M]
Y_N : Nitrogen source cellular yield, [M/M]

Symbols

ρ_h : Hyphae density, [M/L^3] [$1.1´10^{-9}$ $mg.\mu m^{-3}$]
μ : Growth specific rate, [1/T]
μ_{max} : Maximum growth specific rate, [1/T]
φ : Branching frequency, [1/T]
δ_g : Thickness of the gas film, [L]
ε_R : Bed void fraction
γ : Branching proportionality constant
β : Principal hyphae fraction

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