



Packed bed dynamics during microbial treatment of wastewater: Modelling and simulation

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Received 9 April 2007; received in revised form 6 July 2007; accepted 7 July 2007

Available online 21 August 2007

Abstract

A mathematical model consisting of mass balance equations and accounting for bioreaction and mass transfer is presented to describe both unsteady and steady-state degradation of phenol in a biofilter. The model has been validated for the steady-state situation with literature work. The model has been able to predict the dynamics of the biofiltration process with variations in system and operating conditions as inlet substrate concentration, liquid phase mass transfer coefficients, particle size, Henry's constant, inlet velocity, growth and half saturation constants and bed void fraction. The results show that inlet substrate concentration, inlet velocity, growth and half saturation constants and liquid phase mass transfer coefficients significantly control the operational dynamics. It is also shown that inhibition effects can be neglected for low concentrations ($<0.5 \text{ kg m}^{-3}$) of phenol. Thus, the model can be used as a design tool for a biofilter. © 2007 Elsevier Ltd. All rights reserved.

Keywords: Biofiltration; Packed bed; Monod kinetics; Phenol

1. Introduction

Industrial wastes contain compounds that are toxic to human life, aquatic life and others. Most common in them are phenol and chlorophenols. They can cause liver and kidney damage, cardiac toxicity including weak pulse, cardiac depression and reduced blood pressure (Nuhoglu and Yalcin, 2005). The increasing presence of phenols in wastewater represents a significant environmental toxicity hazard. Therefore, the development of methods for removing phenols from industrial wastewater has generated huge interest.

According to the literature, several processes are used to eliminate phenolic compounds from industrial wastewater such as granular or biological activated carbon filtration, ozonation, chlorination, $\text{H}_2\text{O}_2/\text{UV}$ processes, O_3/UV processes, Fenton processes ($\text{Fe}^{2+}/\text{H}_2\text{O}_2$), solvent extraction

and membrane processes. Conventional processes prove to be costly and have the inherent drawbacks due to the tendency of the formation of the secondary toxic materials such as chlorinated phenols (Arutchelvan et al., 2006). The biological treatments have been preferred for the removal of these types of pollutants.

Biofiltration, a potential biological treatment technique is based on the ability of microorganisms (generally bacteria) to convert, under aerobic conditions, organic pollutants to water, carbon dioxide and biomass. Biofiltration is considered as a cost-effective treatment process (Ergas and Cárdenas-González, 2004; Devinny et al., 1999; Ottengraf, 1986; Vazquez et al., 2006). Furthermore, in most of the cases no undesirable by-products or secondary emissions, like in chemical scrubbing or thermal waste gas treatment, are generated (Ergas and Cárdenas-González, 2004; Devinny et al., 1999; Ottengraf, 1986). However, there are still considerable reservations against the use of biofilters, particularly in the United States (Ergas and Cárdenas-González, 2004; Devinny et al., 1999; Zhu et al., 2004). This is possibly due to the difficulty in developing

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accurate mathematical models of the processes involved in biofiltration as a result of non-homogeneity of the packing materials and complexity of the physical, chemical, and microbiological phenomena involved. Furthermore, problems associated with poor and time consuming operation and maintenance procedures and a general lack of understanding of biofiltration with subsequent failures of poorly designed biofilters are the cause of some operators to prefer other treatment options (Streese et al., 2005).

Several authors have developed microkinetic models that attempt to cover all mass transfer and bioconversion processes in the biofilter. The microkinetic model of Ottengraf and van den Oever (1983) is still the most commonly referenced and has been the basis for many other models. It describes a shift from first-order kinetics at low concentrations to zero-order kinetics at high concentrations. Parameters used include Henry's constants, diffusion coefficients, the specific interfacial area per unit volume, and the thickness of the biolayer. The biological degradation is described using Monod kinetics. The models of Shareefdeen et al. (1993) and Zarook et al. (1997) also include the effect of limited oxygen availability. Zarook et al. (1998) considered resident time resolutions diverging from plug flow by implementing a dispersion coefficient. These models (Shareefdeen et al., 1993; Zarook et al., 1997, 1998) regard planar biofilms covering the whole surface of the packing material. In contrast, Shareefdeen and Baltzis (1994) considered partial coverage of the biofilter material by biofilm patches. Direct adsorption to the solid phase not covered with biofilm is described by a Freundlich isotherm. Spigno and Zilli (2004) also presumed partial coverage of the support medium in their model, but did not consider adsorption. However, design of a bioreactor takes into accounts many parameters. None of the above study discussed detailed analysis of the effects of different parameters associated with the models. Moreover, a handy literature for biological treatment of volatile organic compounds (VOCs) is available but a considerable amount of research needs to be done particularly for liquid waste treatment using packed bed reactors.

The parameters considered here are bed height, bed void fraction, particle size, liquid phase mass transfer coefficients, Henry's constant, half saturation constant; inlet

velocity, inlet substrate flow rate and substrate inhibition. In the framework of broader research directed towards the biodegradation of phenol, we have tried to analyze the effects of these parameters on the dynamics of the process for phenol removal. As far as is known, adequate information on specific study on the aerobic degradation of phenol with the above-mentioned purpose is not available in literature. A mathematical microkinetic model using the fundamental equations is developed and simulated in order to predict the behaviour of microorganisms, and to analyze the effects of the above mentioned parameters on the variations of substrate and microorganism concentrations with the operation time and along the bed length. These results would in turn form design basis for engineering purpose.

2. Model development

2.1. Microkinetics

Degradation of phenol in the biofilter is described by a dynamic model based on mass balances considering the mass transfer characteristics of the substrate into the liquid and the biofilm phase and its simultaneous utilization in the biofilm phase. The kinetic model considers oxidation from phenol to carbon dioxide and water, neglecting substrate inhibition effects. Monod kinetics was used to describe the biomass growth kinetics. Therefore, the rate expression for biomass growth is given by

$$\frac{dX_b}{dt} = \frac{\mu C_b X_b}{K_s + C_b} \quad (1)$$

where C_b is the biofilm concentration of substrate (g m^{-3}) and X_b is the biomass concentration (g COD m^{-3}). The kinetic parameters used for the model are shown in Table 1. Application of Monod kinetics is the simplest way of describing the microbial activity, which may not be correctly representing the real life microbial behaviour. Therefore, substrate inhibition effect is also studied after incorporating the substrate inhibition coefficient in the rate equation as discussed afterwards. Both the results are compared to comment on the limiting initial substrate concentration up to which the Monod kinetics remains valid.

Table 1
Parameters with values used in simulation

Parameters	Terms and units	Range of values	Base values	References
C_{i0}	Inlet substrate concentration in liquid phase (kg m^{-3})	0.05–50	0.05	Iliuta et al. (2002)
R_p	Particle radius (m)	0.005–0.1	0.03	Iliuta et al. (2002)
ε	Bed void fraction	0.3–0.6	0.45	Iliuta et al. (2002)
K_l	Liquid phase mass transfer coefficient (m s^{-1})	5.55×10^{-2} – 5.55×10^{-6}	5.55×10^{-4}	Iliuta et al. (2002)
V_b	Superficial velocity (m s^{-1})	1.39×10^{-6} – 1.39×10^{-3}	1.39×10^{-3}	Iliuta et al. (2002)
K_s	Substrate half saturation constant (kg m^{-3})	1–50	10	Iliuta et al. (2002)
H	Henry constant	0.25–10.25	10.25	Assumed
μ	Maximum specific growth constant (s^{-1})	4.7×10^{-5} – 95×10^{-5}	95×10^{-5}	Iliuta et al. (2002)
K_b	Biofilm phase mass transfer coefficient (m s^{-1})	10^{-5}	10^{-5}	Iliuta et al. (2002)

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