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# Modeling of a Foamed Emulsion Bioreactor: II. Model Parametric Sensitivity

**Eunsung Kan, Marc A. Deshusses**

Department of Chemical and Environmental Engineering, University of California, Riverside, California 92521; telephone: 919-660-5480; fax: 919-660-5219; e-mail: marc.deshusses@duke.edu

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**ABSTRACT:** The sensitivity of a conceptual model of a foam emulsion bioreactor (FEBR) used for the control of toluene vapors in air was examined. Model parametric sensitivity studies showed which parameters affect the removal of toluene (as model pollutant) in the FEBR the most significantly, and enabled definition of the limits of the process. Detailed examination of the results indicated that the process is highly complex and that both mass transfer and kinetic limitations can coexist in the bioreactor system. These results will help with the optimization of the design and operation of FEBRs.

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**KEYWORDS:** VOC control; air pollution control; modeling; biologically activated foam; parameter sensitivity; bioreactor

## Introduction

Gas phase bioreactors such as biofilters and biotrickling filters are increasingly utilized for air pollution control from stationary sources (Cox and Deshusses, 1998; Devinny et al., 1999; Mpanias and Baltzis, 1998) because they often offer cost effective treatment of dilute waste gas streams. However, their specific volumetric performance is often limited and novel gas phase bioreactors have been explored (Daugulis, 2001; Kan and Deshusses, 2003; Pressman et al., 2000; Vinage et al., 2001; Wang et al., 2006; Yang et al., 2004). We have recently developed a novel high performance bioreactor system called the foamed emulsion bioreactor (FEBR). The FEBR consists of an emulsion of highly active pollutant-degrading microorganisms and a water-immiscible organic phase which is made into a foam with the air being treated (Fig. 1). The foamed reactor concept was used for the biological elimination of toluene as a model volatile organic compound (Kan and Deshusses, 2003, 2005), for the cometabolic biodegradation of TCE vapors (Kan and Deshusses, 2006) and as a reactive chemical scrubber for the elimination of TCE vapors using Fenton's reagent (Kan et al., 2007).

In the first part of this paper (Kan and Deshusses, 2008), a conceptual model that describes toluene fate and transport in the FEBR was presented. For modeling purpose, the FEBR was assumed to be divided into small ideally mixed subdivisions. All model parameters were determined from independent experiments without any further adjustment of the parameters. Then, the model was validated with experimental results obtained at various operating conditions and model simulations of steady state performance demonstrated the usefulness of the model in describing details of the diffusion-reaction processes involved during the biodegradation of pollutant and transfer of oxygen in the FEBR.

In this article, the sensitivity of the FEBR to model parameters and to operating conditions is presented and discussed. Model parametric sensitivity studies are conducted in order to determine which parameters affect the removal of toluene (as model pollutant) in the FEBR the most significantly, and to understand the limits of the process. These results will help with the optimization of the design and operation of FEBRs.

## Parametric Sensitivity Studies

The values of the model parameters listed in Table I were used for the model parametric sensitivity studies. Note that those values were obtained from experiments and that the

Eunsung Kan's present address is Department of Chemical and Petroleum Engineering, United Arab Emirates University, Al-Ain, P.O. Box 17555, United Arab Emirates. Marc A. Deshusses's present address is Department of Civil and Environmental Engineering, 127 Hudson Hall; P.O. Box 90287, Duke University, Durham, NC 27708-0287.

Correspondence to: M.A. Deshusses

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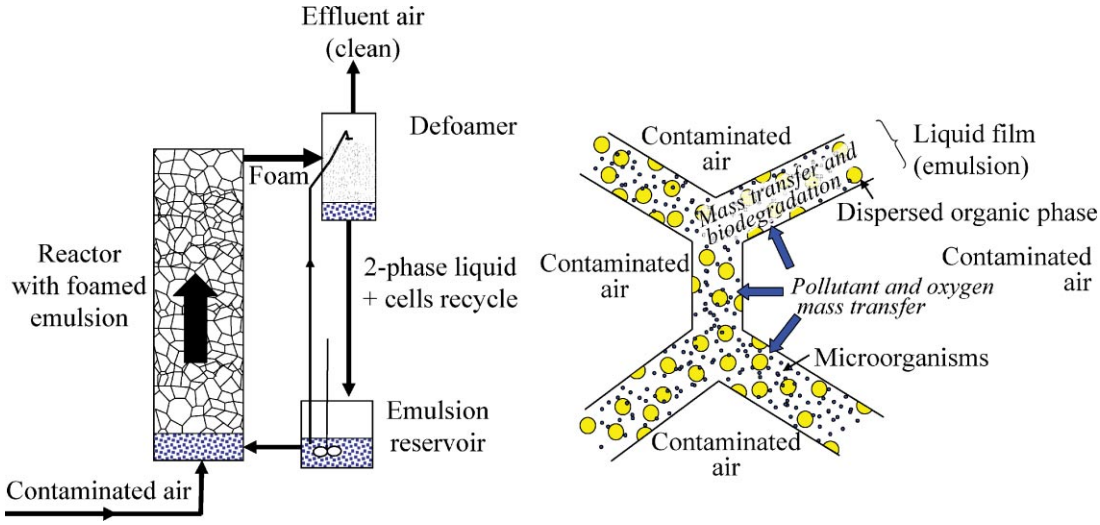


**Figure 1.** Schematic of the FEBR concept (**left**) and structure of the foamed emulsion bubbles (**right**). The liquid film of the foam contains dispersed droplets of organic phase and microorganisms. The foam entraps air with pollutants undergoing treatment. Pollutants and oxygen are transferred to the liquid film where they are degraded (diagrams not to scale). [Color figure can be seen in the online version of this article, available at www.interscience.wiley.com.]

model does not contain any fitted parameters (Kan and Deshusses, 2008). Unless noted otherwise, the sensitivity of toluene removal to model parameters was examined using the following conditions: toluene inlet concentration of 1 g $m^{-3}$, biomass concentration of 16 $g_{dw}$ $L^{-1}$, 3% (v/v) oleyl alcohol concentration, gas retention time of 15 s. The sensitivity of toluene removal to operating parameters was also studied by varying the operating parameters within the range of earlier experimental conditions: 10–40 s for the gas retention time, 0.1–3% (v/v) for oleyl alcohol concentration and 2–16 $g_{dw}$ $L^{-1}$ for biomass concentration. The reader is referred to Part I of the paper for nomenclature of symbols and abbreviations.

## Results and Discussion

The sensitivity of pollutant removal to transport parameters is examined first. The influence of the pollutant diffusion coefficient in the aqueous phase is analyzed in Figure 2. For low diffusion coefficients ($<5 \times 10^{-10}$ $m^2$ $s^{-1}$), a significant decrease of pollutant elimination capacity (EC) is predicted which indicates the presence of a significant diffusion limitation. At higher diffusion coefficients ($>5 \times 10^{-10}$ $m^2$ $s^{-1}$), toluene EC does not depend greatly on the diffusivity, but rather on other parameters such as the maximum biodegradation rate and interphase mass transfer coefficient, indicating a shift from the diffusion limited

**Table I.** Parameters for the FEBR model (see text and Kan and Deshusses, 2008 for details).

| Symbol | Parameter | Numerical value |
|---|---|---|
| $H_{tol,aq}$ | Henry's constant of toluene for air/$H_2O$ | 0.275 (–) |
| $H_{oxy,aq}$ | Henry's constant of oxygen for air/$H_2O$ | 32 (–) |
| $m_{tol}$ | Partition coefficient of toluene between oleyl alcohol and water | 403 (–) |
| $m_{oxy}$ | Partition coefficient of oxygen between oleyl alcohol and water | 2.5 (–) |
| $H_{tol,org}$ | Henry's constant of toluene for air/oleyl alcohol | $6.82 \times 10^{-4}$ (–) |
| $H_{oxy,org}$ | Henry's constant of oxygen for air/oleyl alcohol | 13.2 (–) |
| $D_{tol,aq}$ | Toluene diffusion coefficient in aqueous phase | $3.28 \times 10^{-6}$ ($m^2$ $h^{-1}$) |
| $D_{oxy,aq}$ | Oxygen diffusion coefficient in aqueous phase | $8.58 \times 10^{-6}$ ($m^2$ $h^{-1}$) |
| $D_{tol,org}$ | Toluene diffusion coefficient in oleyl alcohol | $8.8 \times 10^{-8}$ ($m^2$ $h^{-1}$) |
| $D_{oxy,org}$ | Oxygen diffusion coefficient in oleyl alcohol | $2.3 \times 10^{-7}$ ($m^2$ $h^{-1}$) |
| $K_{L,tol}$ | Mass transfer coefficient of toluene between water and oleyl alcohol | 0.01 (m $h^{-1}$) |
| $K_{L,oxy}$ | Mass transfer coefficient of oxygen between water and oleyl alcohol | 0.024 (m $h^{-1}$) |
| $k$ | Maximum biodegradation rate | 0.72 ($g_{toluene}$ $g_{dw}^{-1}$ $h^{-1}$) |
| $K_{m,tol}$ | Half-saturation constant for toluene | 1.77 (g $m^{-3}$) |
| $K_{m,oxy}$ | Half-saturation constant for oxygen | 0.035 (g $m^{-3}$) |
| $Y_{O_2}$ | $O_2$ consumption due to toluene degradation | 1.53 ($g_{O_2}$ $g_{toluene}^{-1}$) |
| $k_{endog}$ | Specific endogenous oxygen uptake rate | 0.06 ($g_{O_2}$ $g_{protein}^{-1}$ $h^{-1}$) |

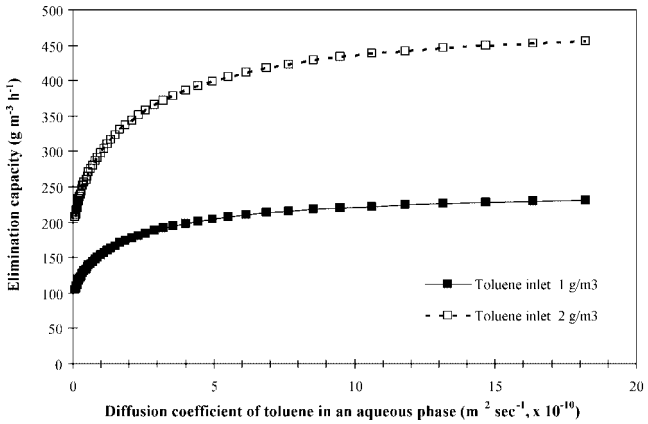


**Figure 2.** Model parametric sensitivity of toluene elimination capacity in the FEBR to the pollutant (toluene) diffusion coefficient and inlet concentration. Conditions for simulation: oleyl alcohol concentration, 3% (v/v); gas residence time, 15 s; biomass concentration, 16 $g_{dw}\,L^{-1}$.

regime. This will be examined and discussed later. At higher pollutant inlet concentrations a greater sensitivity to diffusivity is observed, which is to due to the fact that at the higher loading, the reactor is operated closer to its maximum pollutant elimination capacity.

In Figure 3, the sensitivity of toluene EC to the diffusion coefficient and the specific maximum biodegradation rate $k$ is reported. Figure 3 emphasizes the diffusion limitation predicted for low diffusion coefficients (Fig. 2), and the significant effect of the specific biodegradation rate on pollutant removal when diffusion is not limiting the process. However, there are factors other than degradation rate that limit the process, as indicated by the increase of EC by only about 20–30%, when the biodegradation rate constant is increased by a factor of about 20. This is critical for process optimization since the diffusivity of most volatile organics in pure water is around $10^{-9}$ $m^2\,s^{-1}$. Factors such as the presence of exopolymers will slow down diffusion, while presence of motile bacteria and eddies and fluid motion will increase the effective diffusion coefficient (de Beer et al., 1997; Stewart, 1998, 2003).

Figure 4 reports the sensitivity of toluene EC to the non-aqueous phase (oleyl alcohol) concentration in the emulsion and to the diffusion coefficient of toluene in the aqueous phase. Oleyl alcohol concentration is an important parameter since its presence differentiates the FEBR from single-phase bioactive foam reactors, and many volatile organics have a high partition in oleyl alcohol (e.g., toluene's dimensionless air-oleyl alcohol partition coefficient is 403 compared to 0.275 for air–water). Increasing oleyl alcohol concentration increases the toluene elimination capacity. This is because oleyl alcohol affects the mass transfer of toluene in the system, including gas–liquid absorption of gaseous toluene and partitioning of toluene between the aqueous and organic phase. At the same time, the effect of toluene diffusivity in the aqueous phase is shown. The lines on Figure 4 are slightly concave, indicating that the performance of the FEBR is more sensitive to oleyl alcohol at low oleyl alcohol concentration. This is more pronounced if the diffusion coefficient of the pollutant treated is high, that is, if factors other than diffusion in aqueous phase become somewhat limiting. But, this effect is subtle, which indicates that both oleyl alcohol concentration and pollutant diffusion coefficient have key roles in determining overall mass transfer of pollutant in the FEBR and thus in the performance of the reactor.

The parametric sensitivity of the pollutant elimination capacity to the half-saturation constant ($K_m$) and the oxygen half-saturation constant ($K_o$) is illustrated using toluene

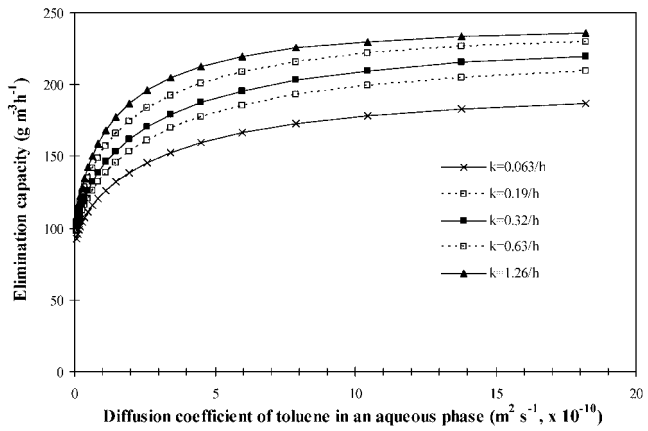


**Figure 3.** Parametric sensitivity of toluene elimination capacity to the diffusion coefficient ($D$) and the maximum specific biodegradation rate ($k$). Conditions for simulation: toluene inlet concentration, 1 $g\,m^{-3}$; oleyl alcohol concentration, 3% (v/v); gas residence time, 15 s; biomass concentration, 16 $g_{dw}\,L^{-1}$.

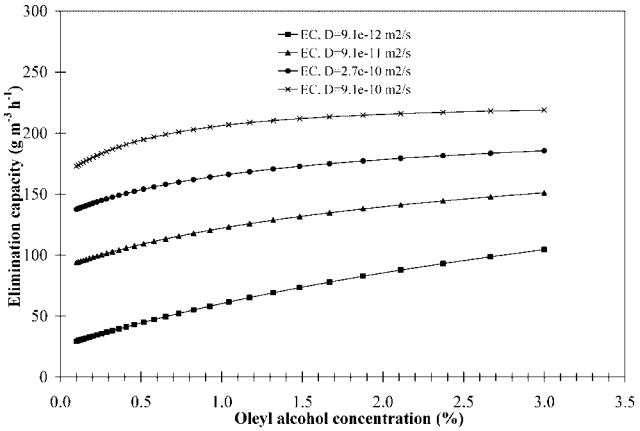


**Figure 4.** Model parametric sensitivity to oleyl alcohol concentration and the diffusion coefficient in the aqueous phase. Conditions for simulation: toluene inlet concentration, 1 $g\,m^{-3}$; gas residence time, 15 s; biomass concentration, 16 $g_{dw}\,L^{-1}$; FEBR height, 0.4 m.

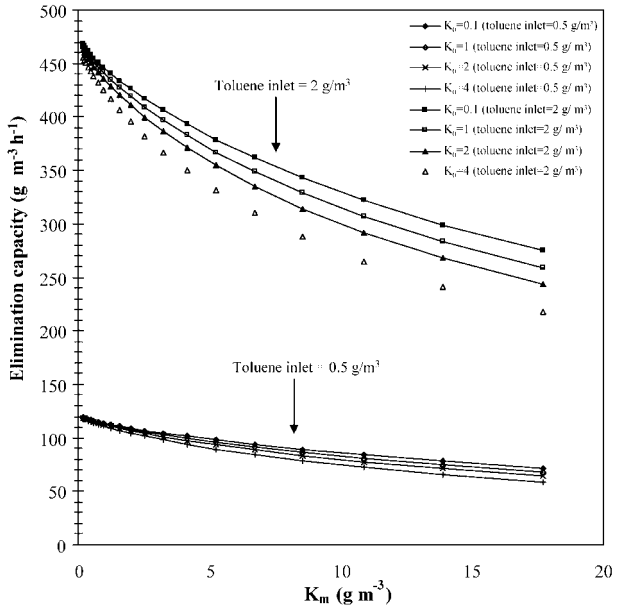


**Figure 5.** Parametric sensitivity of the toluene elimination capacity to the toluene half-saturation constant ($K_m$) and the oxygen half-saturation constant ($K_o$) at two different toluene inlet concentrations. Conditions for simulation: oleyl alcohol concentration, 3% (v/v); gas residence time, 15 s; biomass concentration, 16 $g_{dw}\,L^{-1}$.

as a model pollutant at two different inlet concentrations (0.5 and 2 $g\,m^{-3}$) in Figure 5. At both toluene inlet concentrations, the toluene EC at fixed $K_o$ values decreases when increasing $K_m$. This is because increasing $K_m$ means reducing the affinity of the bacteria for toluene and because in all cases shown in Figure 5, the FEBR is subject to some degree of kinetic limitation. Similarly, the toluene elimination capacity at fixed $K_m$ values decreases as $K_o$ increases when the affinity of bacteria for oxygen is decreased. The effect of $K_o$ is more pronounced at a toluene inlet concentration of 2 $g\,m^{-3}$ than at a toluene inlet concentration of 0.5 $g\,m^{-3}$. This is because the higher toluene concentration requires more oxygen for biodegradation, hence it results in oxygen limiting conditions.

The sensitivity of other parameters was also studied. Unlike the above parameters, it was found that the mass transfer coefficient ($K_L$) of toluene between the aqueous and organic phases in the foam is not a sensitive parameter (results not shown). This came as a surprise as other studies in biphasic reactors had shown that interphase mass transfer limitations often existed (Cruickshank et al., 2000; Marcelis et al., 2003). However, those studies were all considering relatively well mixed biphasic systems, hence the significant diffusion limitation predicted in the FEBR was not present in these well mixed reactors. Another reason for the low sensitivity to $K_L$ is that a relatively high interphase mass transfer rate is possible due to the large interfacial area between the aqueous and organic phases, which diminishes the sensitivity to $K_L$. This is accentuated by the fact that toluene does not penetrate much into the liquid film of the foam because of diffusion limitation.

The sensitivity of the FEBR performance to selected operating parameters is presented in Figures 6–9. These figures allow one to better understand the effect of a given parameter on the FEBR process and to define the limits and possibilities of FEBRs. The operating parameters are biomass concentration, oleyl alcohol concentration and gas retention time. Varying these parameters results in complex effects on gas–liquid mass transfer of pollutant and oxygen, on mass transfer between the aqueous and organic phases, as well as on the biodegradation. Varying the gas velocity also impacts the foam size and the liquid holdup in the FEBR (see Part I of this article). Modeling provides an effective means to understand these complex effects. First, the effect of gas velocity is discussed. The simulated toluene elimination capacity and removal efficiency are plotted in Figure 6. As discussed in Part I of this paper (Kan and Deshusses, 2008), when the gas velocity is varied, the foam characteristics are changed, and therefore the fate and transport of toluene and oxygen in the system change. However, the main effect of changing the gas velocity (at a fixed bed height) is that it changes the gas residence time in the reactor. At low gas velocities, removal is essentially complete, and the elimination capacity increases linearly with increasing the gas velocity, that is, the loading to the system. When the gas velocity reaches about 1.2 m $min^{-1}$, which corresponds to a gas residence time of 20 s in a 40 cm tall FEBR, a significant breakthrough of toluene is predicted and toluene elimination capacity starts to deviate from its linear trend, with corresponding decreases in the removal efficiency. The EC levels off at the maximum elimination capacity of the system, for the given conditions, which in this case is predicted to be about 320 $g\,m^{-3}\,h^{-1}$. A detailed examination of model data (not shown) reveals that at low gas velocities, there is little penetration of toluene in the liquid film and along the reactor height, and complete removal of toluene occurs close to the gas inlet port of the reactor. As the gas

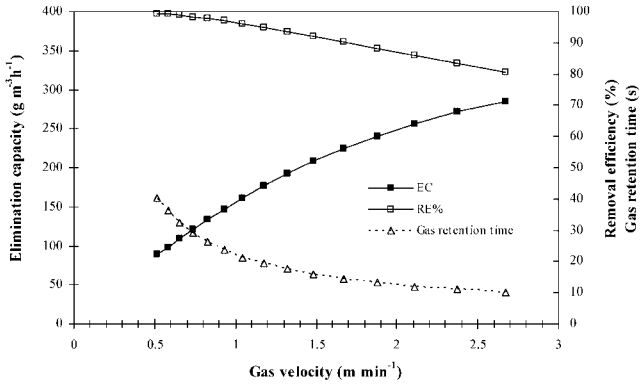


**Figure 6.** Simulation of removal efficiency and elimination capacity at various gas velocity. Conditions for simulation: toluene inlet concentration, 1 $g\,m^{-3}$; oleyl alcohol concentration, 3% (v/v); biomass concentration, 16 $g_{dw}\,L^{-1}$.

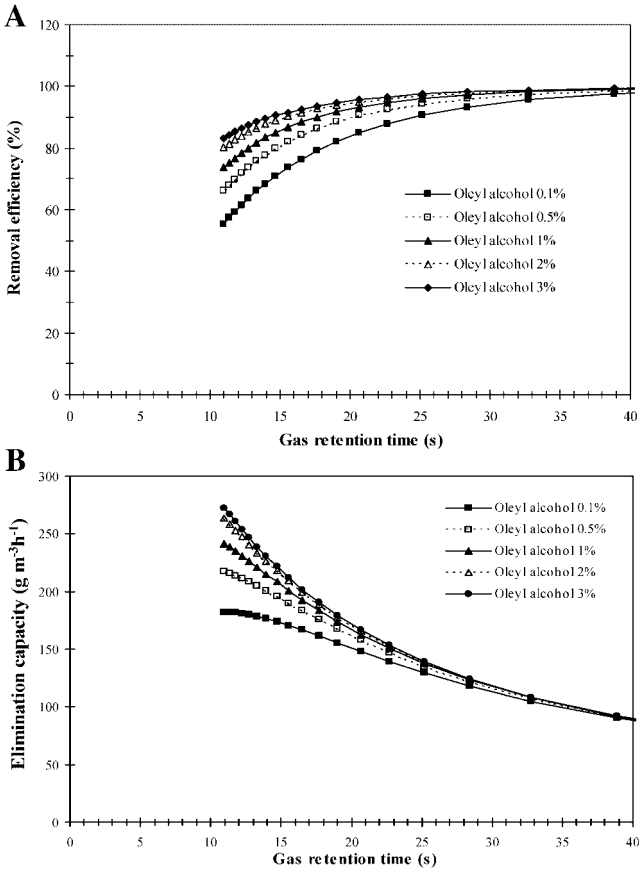


**Figure 7.** Parametric sensitivity of the FEBR to gas retention time and oleyl alcohol concentration. Conditions for simulation: toluene inlet concentration, 1 g $m^{-3}$; biomass concentration, 16 $g_{dw}\,L^{-1}$.

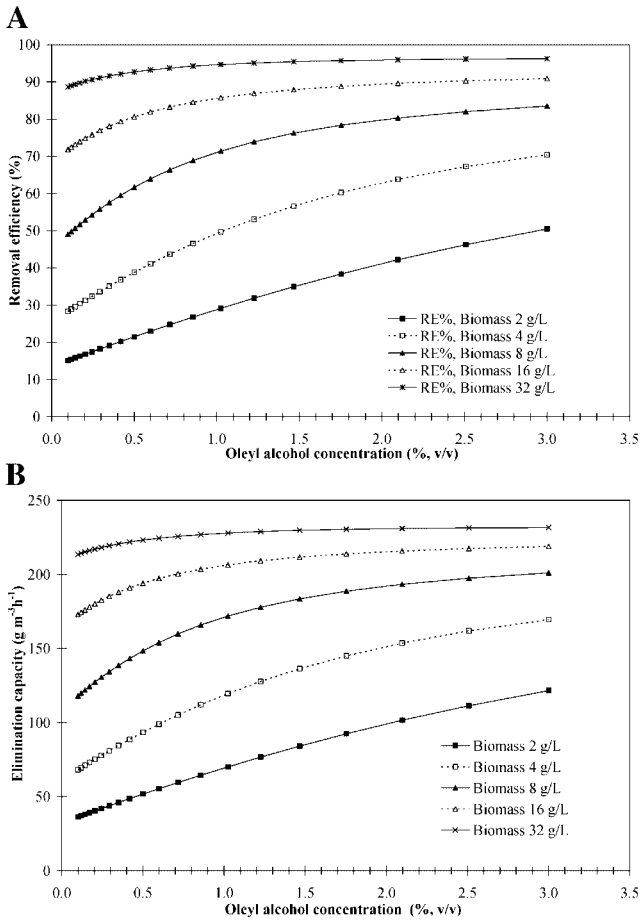


**Figure 8.** Parametric sensitivity of the FEBR to oleyl alcohol concentration and biomass concentration. Conditions for simulation: toluene inlet concentration, 1 g $m^{-3}$; gas retention time, 15 s.

velocity is increased, there is greater penetration of toluene in the film, and greater saturation of the biodegradation kinetics, and only partial removal of toluene. At the highest gas velocities, that is, lowest gas residence times, the process is essentially limited by the biological kinetics, though mass transfer effects are also seen as shown in Figure 7, where toluene removal and EC are plotted versus the gas residence time, for different oleyl alcohol concentrations. This figure illustrates that at low gas residence time, oleyl alcohol plays an important role in increasing the rate of mass transfer, and thereby allowing greater degradation of the pollutant. At the higher gas residence time, toluene removal is essentially complete and the role of oleyl alcohol is diminished.

Figure 8 further explores the effect of oleyl alcohol concentration in conjunction with the effect of biomass concentration. First, it is clear from Figure 8 that biomass concentration plays an important role, as it directly correlated with the degradation capacity of the system. Small change in biomass concentration below 8 $g_{dw}\,L^{-1}$ have drastic effects, while the sensitivity to biomass concentrations decreases as biomass concentration approaches 16 $g_{dw}\,L^{-1}$ which was the value used in most experiments (Kan and Deshusses, 2003). There is also an acceleration of toluene and oxygen mass transfer due to the consumption of pollutant and oxygen by bacteria at or near the gas interface. Also shown in Figure 8 is the effect of oleyl alcohol. At 16 $g_{dw}\,L^{-1}$, the process is relatively insensitive to oleyl alcohol concentration. As biomass concentration decreases, the overall sensitivity to oleyl alcohol increases. This is particularly apparent at the lowest biomass concentration of 2 $g_{dw}\,L^{-1}$ for which there is a quasi linear relationship between pollutant elimination and oleyl alcohol concentration. The reason for this is that at the lowest biomass concentrations, there is a greater penetration of the pollutant into the liquid film as well as axially into the reactor, and greater distribution of the pollutant into the non-aqueous phase. Under these circumstances, the process becomes very sensitive to concentration of oleyl alcohol.

Finally, the sensitivity of the FEBR to biomass concentration and gas retention time is illustrated in Figure 9. As discussed above, decreasing biomass concentration has several effects on the process. First, it decreases the toluene gradient near the liquid–gas interface, and therefore will

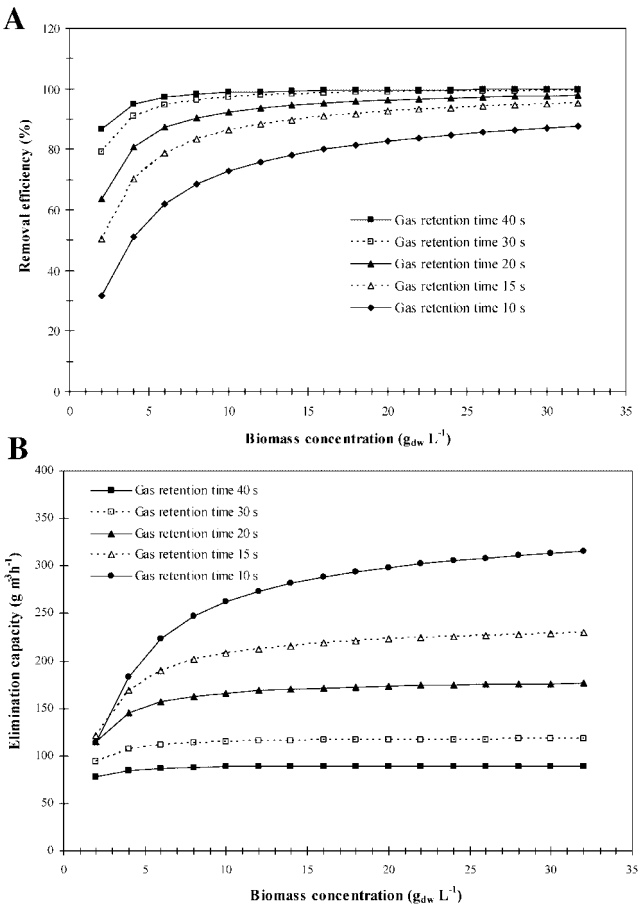


**Figure 9.** Parametric sensitivity of the FEBR to biomass concentration and gas retention time. Conditions for simulation: toluene inlet concentration, 1 g $m^{-3}$; oleyl alcohol concentration, 3% (v/v).

decrease the rate of toluene gas–liquid mass transfer. Second, as biomass concentration decreases, there is a point where too little pollutant is degraded in the liquid film, and full penetration of the pollutant into the liquid film occurs. Both these phenomena will result in a lower rate of pollutant removal from the system, as indicated by the rapid drop in performance in Figure 9 as biomass concentration decreases. On the other hand, at high biomass concentrations, removal is nearly complete (Fig. 9A) and the elimination capacity only depends on the loading to the system.

## Conclusions

The parametric sensitivity of a conceptual mathematical model of a FEBR was examined. The model allowed quantitative description of gas–liquid interphase mass transfer of both oxygen and toluene, detailed description of diffusion, liquid–liquid mass transfer and biodegradation in the fine liquid films that make up the foam bioreactor. Overall, the model simulations allowed description of the behavior of the FEBR over a wide spectrum of operating conditions. Detailed examination of the results indicated that the process is highly complex and that both mass transfer and kinetic limitations can coexist in the reactor system. The model simulations also allowed to define the limits of the process. The detailed understanding of the process gained from such study can be used in optimizing both the reactor design and the operating conditions of FEBRs.

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