

Mathematical Modelling of a Trickle Bed Bioreactor for the removal of H_2S and CS_2

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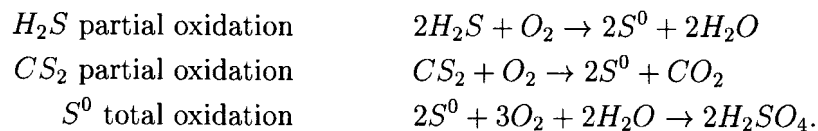
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Report by S. J. Chapman

1 Problem Description

The problem concerned the removal of pollutants from gaseous streams emerging from an industrial process. In this case, the removal of H_2S and CS_2 from air is accomplished by means of a bioreactor with supported micro-organisms. The pollutants are first absorbed in water, and then they are transported to the biofilm where the micro-organisms transform them. The process is shown schematically in Figure 1.

It is believed that the following global reactions take place in the biofilm:



2 Reactor Model

The following model, representing mass conservation of each species in the gas, liquid and biofilm phases, was brought to the study group.

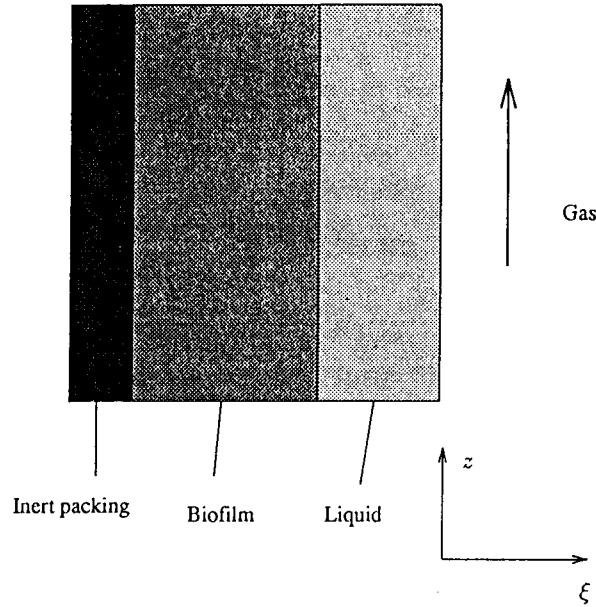


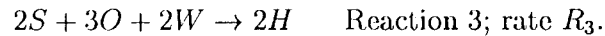
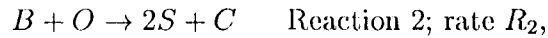
Figure 1: Schematic diagram of the bioreactor.

Reactions: The important species are labelled as follows:

$$A = H_2S; \quad B = CS_2; \quad C = CO_2;$$

$$H = H_2SO_4; \quad O = O_2; \quad S = S; \quad W = H_2O.$$

The reactions may then be written:



Under the assumptions that the gas and liquid phases are in plug flow, diffusion is negligible in both gas and liquid phases by comparison to convection except in boundary layers, and diffusion in the z -direction is negligible in the bioreactor, the following conservation equations were proposed:

Gas Phase

$$-u_G \frac{\partial C_{AG}}{\partial z} - (k_L a)_A (H_A C_{AG} - \bar{C}_{AL}) = \frac{\partial C_{AG}}{\partial t}, \quad (1)$$

$$-u_G \frac{\partial C_{BG}}{\partial z} - (k_L a)_B (H_B C_{BG} - \bar{C}_{BL}) = \frac{\partial C_{BG}}{\partial t}. \quad (2)$$

Liquid Phase

$$-\bar{u}_L \frac{\partial \bar{C}_{AL}}{\partial z} + (k_L a)_A (H_A C_{AG} - \bar{C}_{AL}) - (k_p a)_A (\bar{C}_{AL} - C_{AL,i}) = \frac{\partial \bar{C}_{AL}}{\partial t}, \quad (3)$$

$$-\bar{u}_L \frac{\partial \bar{C}_{BL}}{\partial z} + (k_L a)_B (H_B C_{BG} - \bar{C}_{BL}) - (k_p a)_B (\bar{C}_{BL} - C_{BL,i}) = \frac{\partial \bar{C}_{BL}}{\partial t}, \quad (4)$$

$$-\bar{u}_L \frac{\partial \bar{C}_{OL}}{\partial z} + (k_L a)_O (H_O C_{OG} - \bar{C}_{OL}) - (k_p a)_O (\bar{C}_{OL} - C_{OL,i}) = \frac{\partial \bar{C}_{OL}}{\partial t}. \quad (5)$$

Biofilm Phase

$$D_A \frac{\partial^2 C_{AP}}{\partial \xi^2} + \alpha_{A1} R_1 = \frac{\partial C_{AP}}{\partial t}, \quad (6)$$

$$D_B \frac{\partial^2 C_{BP}}{\partial \xi^2} + \alpha_{B2} R_2 = \frac{\partial C_{BP}}{\partial t}, \quad (7)$$

$$D_O \frac{\partial^2 C_{OP}}{\partial \xi^2} + \alpha_{O1} R_1 + \alpha_{O2} R_2 + \alpha_{O3} R_3 = \frac{\partial C_{OP}}{\partial t}. \quad (8)$$

Here C_{mG} , \bar{C}_{mL} , C_{mP} and $C_{mL,i}$, represent the concentration of compound m in the gas phase, the average concentration in the liquid phase, the concentration in the biofilm, and the concentration on the liquid/biofilm interface respectively; u_G is the velocity of the gas, \bar{u}_L is the average velocity of the liquid, D_m is the diffusion coefficient for compound m in the biofilm, the (ka) are mass transfer coefficients, and $\alpha_{m,n}$ is the stoichiometric coefficient for compound m in reaction n (positive for products, negative for reactants). Distance down the reactor is denoted by z , and distance across denoted by ξ .

These equations are supplemented by suitable initial conditions and entrance conditions on the concentrations in the liquid and gas phases (i.e. conditions at $z = 0$). Furthermore, the following boundary conditions were proposed for the biofilm:

$$\text{At } \xi = 0 \quad (k_p a)_A (\bar{C}_{AL} - \bar{C}_{AL,i}) = -D_A \frac{\partial C_{AP}}{\partial \xi}, \quad (9)$$

$$(k_p a)_B (\bar{C}_{BL} - \bar{C}_{BL,i}) = -D_B \frac{\partial C_{BP}}{\partial \xi}, \quad (10)$$

$$(k_p a)_O (\bar{C}_{OL} - \bar{C}_{OL,i}) = -D_O \frac{\partial C_{OP}}{\partial \xi}, \quad (11)$$

Gas velocity	u_G	40 cm s ⁻¹
Liquid velocity	\bar{u}_L	10 cm s ⁻¹
Diffusion coefficient in liquid	D_L	10 ⁻⁵ cm ² s ⁻¹
Diffusion coefficient in gas	D_G	10 ⁻¹ cm ² s ⁻¹
Concentration in liquid	C_L	5.6 × 10 ⁻² mol cm ⁻³
Length of bioreactor	l	500 cm
Width of gas phase	d_G	100 cm
Width of liquid phase	d_L	10 ⁻² cm
Henry's constant	H	2.5 × 10 ⁻²
Mass transfer coefficient	k_L	4 × 10 ⁻³ cm s ⁻¹
Surface/Volume ratio	a	2.15 cm ⁻¹
Mass transfer coefficient	$(k_L a)$	8.3 s ⁻¹

Table 1: Typical values of parameters relevant to the bioreactor.

$$\text{At } \xi = \delta_A \quad \frac{\partial C_{AP}}{\partial \xi} = 0, \quad (12)$$

$$\text{At } \xi = \delta_B \quad \frac{\partial C_{BP}}{\partial \xi} = 0, \quad (13)$$

$$\text{At } \xi = \delta_O \quad \frac{\partial C_{OP}}{\partial \xi} = 0. \quad (14)$$

Here $\delta_m(t)$ represents the distance into the biofilm over which the microorganisms are actively consuming compound m , and evolves according to the law

$$\frac{d\delta_m}{dt} = - \left(\frac{\partial C_{mP}/\partial t}{\partial C_{mP}/\partial \xi} \right)_{\xi=\delta_m}. \quad (15)$$

Typical values for the parameters appearing these equations are shown in Table 1.

This model has been implemented numerically by R. Lobo. However, it was found that when realistic values for each constant were taken, that the model predicted that only 0.01 percent of the pollutant would be removed from the gas stream.

The problem posed at the study group was to determine whether this was due to an error in the coding, or an error in the modelling. If the modelling was found to be at fault, then the study group was asked to suggest which important physical mechanisms may have been left out of the model, and

to determine the likely effect these would have. In particular, Mr. Lobo suggested that some of the micro-organisms may find their way into the liquid phase, and so it may be necessary to include some reaction taking place in the liquid. The study group was asked to determine whether this would be enough to account for the difference between the observed and predicted behaviour of the bioreactor.

3 Simplified model

The concentrations of compounds A , B and O are coupled only through the rates of the reactions in the biofilm. For simplicity, we consider the case when there is only a single compound, A , say. We will also only consider the situation in which the reactor is operating in a steady state. This gives the following simplified model, in which we have dropped the subscript A :

$$\text{Gas Phase:} \quad -u_G \frac{\partial C_G}{\partial z} - (k_L a)(HC_G - \bar{C}_L) = 0, \quad (16)$$

$$\text{Liquid Phase:} \quad -\bar{u}_L \frac{\partial \bar{C}_L}{\partial z} + (k_L a)(HC_G - \bar{C}_L) - (k_P a)(\bar{C}_L - C_{L,i}) = 0, \quad (17)$$

$$\text{Biofilm Phase:} \quad D \frac{\partial^2 C_P}{\partial \xi^2} + R = 0, \quad (18)$$

where the reaction rate R is supposed to depend only on the concentration C_P .

Since $\bar{C}_L \geq 0$, a bound on the mass transfer between the gas and liquid phases can be obtained by setting $\bar{C}_L = 0$ in equation (16). This gives a very simple check on the numerical solution obtained by V. Lobo. With \bar{C}_L set to zero, equation (16) becomes

$$-u_G \frac{\partial C_G}{\partial z} - (k_L a)HC_G = 0, \quad (19)$$

with solution

$$C_G = C_G^0 \exp(-k_L a H z / u_G). \quad (20)$$

Thus we find that the length scale for the decay of the concentration in the gas is given by $u_G / (k_L a) H$, which for the values given in Table 1 turns out to be approximately 2000m. Since the reactor is only about 5m long, this explains the extremely small change in concentration observed in the numerical

solution. Note that even adding a reaction in the liquid to the model (16)-(18), would not solve the problem, since we can never have the concentration in the liquid lower than zero. It seems that the mass transfer coefficient ($k_L a$) is just too small for the pollutants to have time to be absorbed into the liquid.

Mass transfer by diffusion The mass transfer law in equation (16) is an approximation to the local diffusive mass transfer between the liquid and gas phases. We can check that the value of ($k_L a$) given is of the right order of magnitude by considering a local diffusion problem at the gas/liquid interface.

Since we are aiming only to verify the order of magnitude of ($k_L a$), we will consider the simpler case of a co-current (rather than counter-current) reactor. We ignore the effects of the finite thickness of the liquid and gas films, and consider an infinite stream of gas moving parallel to an infinite stream of liquid, with pollutant diffusing from the gas to the liquid. Thus we are assuming that diffusion is important only in a thin layer near the interface. We will return to this point later.

This gives us the following test problem:

$$D_L \frac{\partial^2 C_L}{\partial \xi^2} = \bar{u}_L \frac{\partial C_L}{\partial z}, \quad \xi < 0, \quad (21)$$

$$D_G \frac{\partial^2 C_G}{\partial \xi^2} = \bar{u}_G \frac{\partial C_G}{\partial z}, \quad \xi > 0, \quad (22)$$

with boundary conditions

$$H C_G = C_L \quad \text{on } \xi = 0, \quad (23)$$

$$D_L \frac{\partial C_L}{\partial \xi} = D_G \frac{\partial C_G}{\partial \xi} \quad \text{on } \xi = 0, \quad (24)$$

$$C_L \rightarrow 0 \quad \text{as } \xi \rightarrow -\infty, \quad (25)$$

$$C_G \rightarrow C_G^0 \quad \text{as } \xi \rightarrow \infty, \quad (26)$$

$$C_L = 0 \quad \text{on } z = 0, \quad (27)$$

$$C_G = C_G^0 \quad \text{on } z = 0. \quad (28)$$

Equation (23) is Henry's law for equilibrium at the interface, and equation (24) represents conservation of pollutant at the interface.

Equations (21)-(28) have the following similarity solution:

$$C_L = A \sqrt{\frac{2D_L}{\bar{u}_L}} \int_0^{\frac{\xi}{\sqrt{z}}} \sqrt{\frac{\bar{u}_L}{2D_L}} e^{-s^2/2} ds + BH, \quad (29)$$

$$C_G = A \frac{D_L}{D_G} \sqrt{\frac{2D_L}{\bar{u}_L}} \int_0^{\frac{\xi}{\sqrt{z}}} \sqrt{\frac{\bar{u}_L}{2D_L}} e^{-s^2/2} ds + B, \quad (30)$$

where

$$A = \frac{HC_G^0/\sqrt{\pi}}{\left((D_L/D_G)H\sqrt{D_G/\bar{u}_G} - \sqrt{D_L/\bar{u}_L} \right)}, \quad (31)$$

$$B = \frac{C_G^0}{1 - H\sqrt{\bar{u}_L D_L/\bar{u}_G D_G}}. \quad (32)$$

For the values of the parameters given in Table 1, $A \sim -2 \times 10^2 C_G^0$, $B \sim C_G^0$. The flux of pollutant, q , across the interface $\xi = 0$ is given by

$$q = D_L \frac{\partial C_L}{\partial \xi} = \frac{AD_L}{\sqrt{z}} \sim 10^{-4} C_G^0 \text{ cm s}^{-1}.$$

The flux the problem (19) was given by

$$q = k_L H C_G \sim 10^{-4} C_G^0 \text{ cm s}^{-1}.$$

Thus we conclude that the mass transfer coefficient ($k_L a$) is of the right order of magnitude when based on a local diffusive mass transfer mechanism.

In the solutions (29), (30) we note that

$$A \sqrt{\frac{2D_L}{\bar{u}_L}} \sim 0.34 C_G^0, \quad A \frac{D_L}{D_G} \sqrt{\frac{2D_L}{\bar{u}_L}} \sim 1.4 \times 10^{-3} C_G^0.$$

Thus we see that the concentration in the liquid is varying significantly, even though the concentration in the gas is hardly changing. This would seem to imply that diffusion is not important in the gas phase, but it is important in the liquid phase.

We can estimate the relative importance of diffusion and convection by considering the following non-dimensional diffusion coefficient:

$$\bar{D} = \frac{\text{diffusion}}{\text{convection}} = \frac{Dl}{d^2 \bar{u}},$$

where d is the thickness of the region and l is its length. We find that in the gas phase $\bar{D} = 10^{-4}$, so that convection dominates, whereas in the liquid phase $\bar{D} = 5$, and diffusion is at least as important as convection. This draws into question the neglect of diffusion in equations (3)-(5).

The large non-dimensional diffusion coefficient in the liquid phase also means that the assumption that diffusion is important only in a thin layer near the interface is wrong. However, the small non-dimensional diffusion coefficient in the gas phase means that the concentration in the gas phase is only a function of z . There is one more simple test problem we can use to check whether this affects the mass transfer coefficient ($k_L a$). We consider the diffusion problem in the liquid phase, now taken to be of finite width. We assume that the biofilm is performing perfectly, so that the concentration of pollutant is zero on the interface between the liquid and the biofilm. We assume that the concentration in the gas phase is held fixed at C_G^0 . This, again, will give a best possible estimate for the mass transfer coefficient. We arrive at the following problem:

$$D_L \frac{\partial^2 C_L}{\partial \xi^2} = \bar{u}_L \frac{\partial C_L}{\partial z}, \quad 0 < \xi < d_L, \quad (33)$$

$$C_L = 0 \quad \text{on } \xi = 0, \quad (34)$$

$$C_L = HC_G^0 \quad \text{on } \xi = d_L, \quad (35)$$

$$C_L = 0 \quad \text{on } z = 0. \quad (36)$$

Equations (33)-(36) have the following Fourier series solution:

$$C_L = HC_G^0 \left(\frac{x}{d_L} + \sum_{n=1}^{\infty} \frac{2(-1)^n}{n\pi} e^{-\frac{n^2 \pi^2 D_L z}{d_L^2 \bar{u}_L}} \sin \frac{n\pi \xi}{d_L} \right). \quad (37)$$

The flux through the gas/liquid interface is given by

$$q = D_L \frac{\partial C_L}{\partial \xi} = HC_G^0 \left(\frac{D_L}{d_L} + D_L \sum_{n=1}^{\infty} \frac{2}{d_L} e^{-\frac{n^2 \pi^2 D_L z}{d_L^2 \bar{u}_L}} \right).$$

With the values given in Table 1 the decay rate of the exponentials is given by

$$\frac{\pi^2 D_L}{d_L^2 \bar{u}_L} \sim 10^{-1} \text{ cm.}$$

Thus, once z is greater than about 10 cm the profile in the liquid is approximately linear, and the flux is given by

$$q \sim 10^{-4} C_G^0 \text{ cm s}^{-1}.$$

The linear profile in the liquid means that it is working to capacity, and yet the flux is still too small.

Capacity The capacity of a mass (or heat) exchanger is defined as

$$C = \frac{\text{amount of pollutant liquid can hold in equilibrium}}{\text{amount of pollutant gas can hold in equilibrium}}.$$

Clearly this number should be as large as possible for efficient exchange, and in particular it is useful for it to be greater than unity. For the bioreactor under consideration

$$C = \frac{H\bar{u}_L d_L}{\bar{u}_G d_G} \sim 0.6 \times 10^{-6}.$$

This extremely low capacity is due to the low solubility of the pollutant in the liquid and the high speed of the gas stream, and is the reason for the extremely low mass transfer coefficient. Indeed, it is this low capacity which requires the use of the micro-organisms in the first place. However, before the micro-organisms can get to work the pollutants need to be transported to them across the liquid film. From our calculations thus far it appears that diffusion alone is not powerful enough to transport sufficient quantities across the liquid film.

Reaction in the Liquid Whereas including a reaction term in equation (17) would not lead to much more pollutant being extracted from the gas phase, including a reaction in the liquid phase in equation (33) would have a greater effect, since the reaction would decrease the amount of pollutant in the liquid, increasing the gradient at the boundary and thus increasing the mass transfer (including a reaction here effectively reduces the width of the liquid film).

Since we have seen that the liquid phase was previously diffusion dominated (the solution (37) approaches a linear profile within about 10 cms)

we consider here a problem in which the diffusion across the liquid phase is enhanced by a reaction there also. Thus we have:

$$D_L \frac{\partial^2 C_L}{\partial \xi^2} = RC_L, \quad 0 < \xi < d_L, \quad (38)$$

$$C_L = 0 \quad \text{on } \xi = 0, \quad (39)$$

$$C_L = HC_G^0 \quad \text{on } \xi = d_L. \quad (40)$$

Setting $R = 0$ gives the linear profile found previously. With nonzero constant R the solution is

$$C_L = \frac{HC_G^0}{\sinh d_L \sqrt{R/D_L}} \sinh \xi \sqrt{R/D_L}. \quad (41)$$

The flux through the liquid/gas interface is given by

$$q = D_L \frac{\partial C_L}{\partial \xi} = HC_G^0 \sqrt{D_L R} \coth d_L \sqrt{R/D_L} \sim 10^{-4} \sqrt{R} C_G^0 \text{ cm s}^{-1/2}.$$

To change the flux by the two orders of magnitude necessary, we require that $R \sim 10^4 \text{s}^{-1}$. Typical values of R in practice are $R \sim 10^{-4} - 10^{-2} \text{s}^{-1}$.

Convection With diffusion transporting pollutant too slowly, and with the reaction in the liquid not quick enough to remove enough pollutant, we are left with convection as the only other possible mechanism for transporting pollutant from the gas to the liquid phase. In order to estimate the effect of slightly non-perfect geometries on the flow fields, we consider the following model problem. Suppose the gas/liquid interface is still given by $\xi = d$, but suppose now that the biofilm/liquid interface is not planar, but given by $\xi = \epsilon h(z)$, where $\epsilon \ll 1$. Assuming the flow of liquid to be irrotational and incompressible, we arrive at the following problem

$$\mathbf{u}_L = \nabla \phi, \quad (42)$$

$$\nabla^2 \phi = 0 \quad \epsilon h(z) < \xi < d_L, \quad (43)$$

$$\mathbf{u}_L \cdot \mathbf{n} = \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \xi = \epsilon h(z), \quad (44)$$

$$\mathbf{u}_L \cdot \mathbf{n} = \frac{\partial \phi}{\partial n} = 0 \quad \text{on } \xi = d_L, \quad (45)$$

where \mathbf{n} represents the unit normal to each interface. We assume that the dominant flow is uniform in the z -direction, and consider the perturbation to this flow induced by the non-planar geometry by expanding \mathbf{u}_L and ϕ in powers of ϵ as follows:

$$\mathbf{u}_L = (0, V_L) + \epsilon \mathbf{u}_1 + \dots, \quad (46)$$

$$\phi = V_L z + \epsilon \phi_1 + \dots. \quad (47)$$

The problem for ϕ_1 is then

$$\nabla^2 \phi_1 = 0 \quad 0 < \xi < d_L, \quad (48)$$

$$\frac{\partial \phi_1}{\partial \xi} = V_L \frac{dh}{dz} \quad \text{on } \xi = 0, \quad (49)$$

$$\frac{\partial \phi_1}{\partial \xi} = 0 \quad \text{on } \xi = d_L. \quad (50)$$

We consider the case in which $h(z) = \sin kz$ (a more general perturbation of the boundary may be built up as a superposition of these Fourier modes). The solution to (48)-(50) is then

$$\phi_1 = -V_L \frac{\cos kz \cosh k(x - d_L)}{\sinh kd_L}, \quad (51)$$

which gives

$$\mathbf{u}_1 = \left(-V_L k \frac{\cos kz \sinh k(x - d_L)}{\sinh kd_L}, V_L k \frac{\sin kz \cosh k(x - d_L)}{\sinh kd_L} \right). \quad (52)$$

Thus the perturbation to the velocity field is of the order $\epsilon k V_L$.

Having solved for the flow field, we may now return to the convection/diffusion problem for the concentration of pollutant. With $\mathbf{u}_L = (u, v)$ we have

$$D_L \frac{\partial^2 C_L}{d\xi^2} = u \frac{\partial C_L}{\partial \xi} + v \frac{\partial C_L}{\partial z} \quad (53)$$

If we suppose that convection is the dominant mechanism, then we have $\mathbf{u} \cdot \nabla C_L = 0$ and the pollutant is convected along streamlines. Since the streamlines do not intersect the boundary diffusion is still the transfer mechanism, but since the streamlines may carry the pollutant some of the way

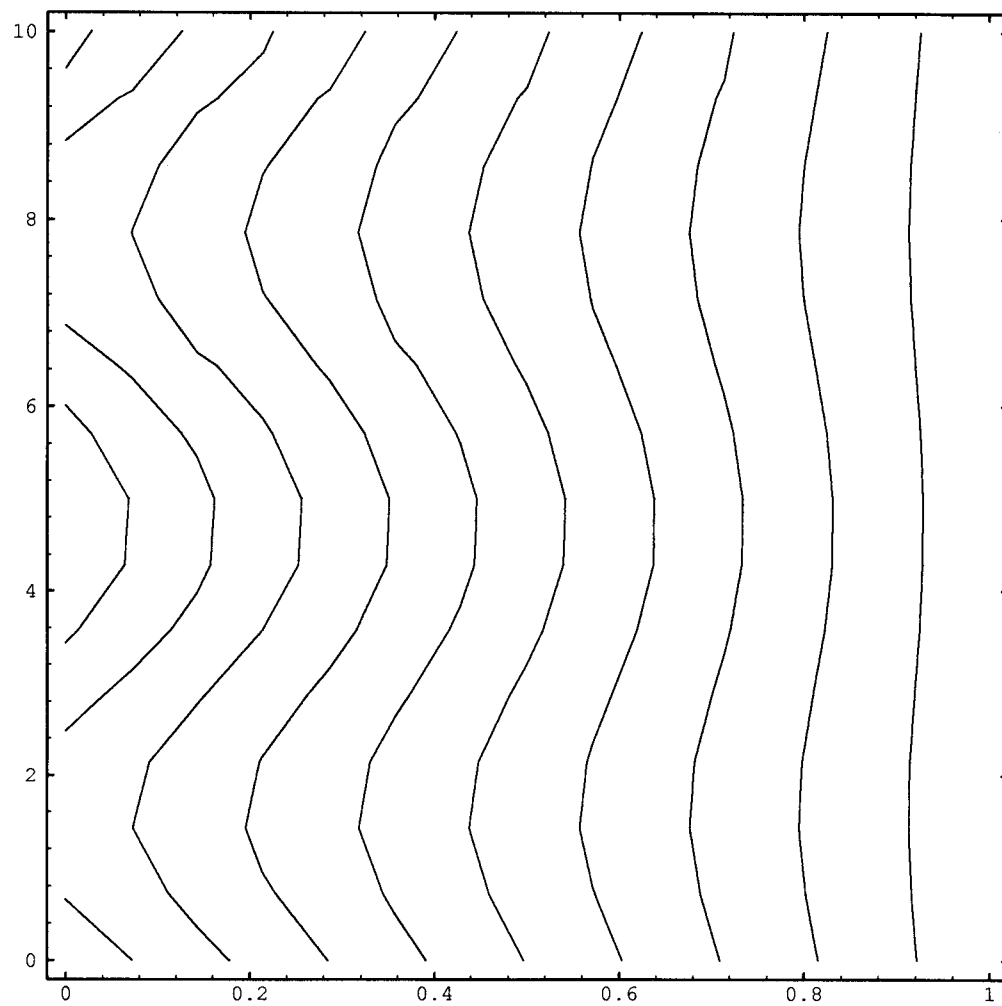


Figure 2: Typical streamlines for the solution (51).

across the liquid phase, the distance to diffuse is smaller. However, convection will only significantly enhance diffusion if streamlines passing near $\xi = d_L$ reach close to $\xi = 0$ in a reasonable distance in the z -direction. Typical streamlines for the solution (51) are shown in Figure 2.

Note that the streamlines near $\xi = d_L$ do not pass close to $\xi = 0$, so that pollutant is still not transported across the film. In order to enhance mass transfer sufficiently we need some mixing in the liquid layer.

The Reynolds number for the liquid flow, based on a vertical velocity of 10 cm s^{-1} and a reactor height of 500 cm , is 5×10^5 . If the bumps on the biofilm are sufficient to generate significant mixing in the liquid layer, then pollutant will be convected across the film, and there will be a diffusive boundary layer of thickness $\delta \sim D_L/u$, with the flux being given by $q = D_L HC_G^0/\delta \sim u HC_G^0$. Hence mixing enhances the mass transfer by a factor of d_L/δ .

To gain two orders of magnitude in mass transfer we require that $\delta/d_L \sim 10^{-2}$, i.e. that $\delta \sim 10^{-4} \text{ cm}$. Since $D_L \sim 10^{-5} \text{ cm}^2\text{s}^{-1}$, we therefore need a horizontal velocity $u \sim 10^{-1} \text{ cm s}^{-1}$. Since $V_L \sim 10 \text{ cm s}^{-1}$, this implies that $\epsilon k \sim 10^{-2}$, that is, we require the amplitude of the bumps on the biofilm to be of the order of 10^{-6} m . This is well within the realms of possibility.

Thus it seems possible that, because of the relatively high velocity of the liquid phase, the stirring induced by a non-planar biofilm/liquid interface will significantly enhance the mass transfer across the liquid film.

Reaction in the Biofilm Including the possibility of mixing in the liquid phase has enhanced the mass transfer coefficient so that the flux of pollutant may approach a realistic value. However, once the pollutant reaches the biofilm, it still needs to be removed by the micro-organisms.

The model proposes a balance between diffusion and reaction in the biofilm, similar to the analysis in the liquid in (38)-(40). In fact, a bound on the rate at which pollutant can be removed can be found by assuming that the liquid does a perfect job of transporting the pollutant to the biofilm, so that the concentration on the liquid/biofilm interface is HC_G^0 . Then the problem in the biofilm is

$$D_B \frac{\partial^2 C_B}{\partial \xi^2} = RC_B, \quad 0 < \xi < d_B, \quad (54)$$

$$\frac{\partial C_B}{\partial \xi} = 0 \quad \text{on } \xi = 0, \quad (55)$$

$$C_B = HC_G^0 \quad \text{on } \xi = d_B, \quad (56)$$

With solution

$$C_B = \frac{HC_G^0}{\cosh d_B \sqrt{R/D_B}} \cosh \xi \sqrt{R/D_B}. \quad (57)$$

The flux through the liquid/biofilm interface is given by

$$q = D_B \frac{\partial C_B}{\partial \xi} = HC_G^0 \sqrt{D_L R} \tanh d_B \sqrt{R/D_L} \sim 10^{-4} \sqrt{R} C_G^0 \text{ cm s}^{-1/2}. \quad (58)$$

As before, an enormous reaction rate is required in order to extract significant amounts of pollutant from the gas.

From the simple model (19), the flux of pollutant from the gas required to decrease the concentration by an order one amount in the length of the reactor is given by

$$q \sim \frac{u_G}{d_{Gl}} C_G^0 \sim 4 \times 10^{-2} C_G^0 \text{ cm s}^{-1}. \quad (59)$$

Hence from (58) we require $R \sim 10^4 \text{ s}^{-1}$. Again, this is an extraordinary high reaction rate.

Reaction in a well mixed liquid phase If we assume that the liquid phase is well mixed, so that the concentration of pollutant is independent of ξ except in diffusive boundary layers, and we also assume that some reaction is taking place, then the amount of pollutant converted is given by $d_L R C_G^0$. Setting this equal to the desired flux gives a required value of R as

$$R \sim 4 \text{ s}^{-1}.$$

The reasons for the reduced value, are (i) that the flux now depends linearly on R rather than on \sqrt{R} since the concentration of pollutant is independent of ξ , and (ii) the reaction takes place throughout the whole film rather than in a thin boundary layer.

4 Conclusion

Flux of pollutant A simple calculation has shown that the flux required to significantly reduce the concentration of pollutant in the gas region is of

the order of

$$q \sim \frac{u_G}{d_{Gl}} C_G^0 \sim 4 \times 10^{-2} C_G^0 \text{ cm s}^{-1}.$$

This large flux is due to the large width of the gas film and its high speed.

With diffusion alone acting as the mass transfer mechanism the flux across the liquid/gas interface was of the order of

$$q \sim \sim 10^{-4} C_G^0 \text{ cm s}^{-1}.$$

Including a reaction in the liquid region enhanced this flux slightly, but the desired flux would require a reaction rate

$$R \sim 10^4 \text{ s}^{-1}.$$

If the liquid layer is assumed to be well mixed rather than laminar, the mass transfer of pollutant across the liquid film is enhanced and approaches a realistic value.

Removal of pollutant Even assuming the pollutant can make its way across the liquid sufficiently quickly, in order to consume the pollutant at the required rate in the biofilm would require a reaction rate there

$$R \sim 10^4 \text{ s}^{-1}.$$

However, if the liquid phase is well mixed rather than laminar flow, so that the concentration is independent of ξ and the reaction takes place uniformly throughout, then the reaction rate required to produce the desired flux is

$$R \sim 4 \text{ s}^{-1}.$$

This reduced rate is due to the reaction taking place throughout the liquid region, rather than in a thin boundary layer.

Finally, we comment on the proposed free boundary in the original model (12)-(14). Such a free boundary is an unnecessary complication in the model, since the effective distance that the biofilm is active will emerge naturally as a length scale in the diffusion problem. We propose this boundary condition be replaced by the simpler fixed condition that the flux of pollutant through the inner biofilm wall is zero.

