Application of the Penetration Theory to Oxygen Transfer to Biofilms

B. E. Logan and S. W. Hermanowicz
Department of Civil Engineering, Division of Sanitary, Environmental, Coastal and Hydraulic Engineering, University of California, Berkeley, Berkeley, California 94720

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In aerobic biological treatment processes using fixed films, such as the trickling filter process, oxygen transport to the biofilm can occur through a moving liquid film. Since many researchers report that process efficiency may be oxygen transport limited, a fundamental model of oxygen transport to biofilms is required before more complex treatment processes can be understood. Although fluid thicknesses typically employed in biofilm models for inclined plates are on the order of several hundred microns, a recent biofilm model by Benefield and Molz considered a 10-cm-thick fluid moving at 322 cm/day over a biofilm. In such cases, fluid flow is laminar and oxygen transport from the air-liquid interface may not reach the biofilm surface. This allows a model of oxygen transfer from the air to the liquid to be uncoupled from a model of oxygen transfer to the biofilm. In the present communication, it is shown that oxygen transport to very thick and slowly moving fluids can be adequately described by penetration theory, and that the completely mixed fluid layer approach used by Benefield and Molz is inappropriate.

OXYGEN TRANSFER FROM AIR TO LIQUID

A general equation describing nonsteady transfer of oxygen into a flowing liquid film is:

\[
\frac{\partial C}{\partial t} = v \frac{\partial C}{\partial z} - D \frac{\partial^2 C}{\partial z^2} \tag{1}
\]

where \(C\) is the concentration of oxygen; \(v\) is the velocity of the fluid; \(D\) is the diffusivity of oxygen through the fluid; \(x\) is the distance from the air-liquid interface; and \(z\) is the distance from the fluid entrance. For Reynolds numbers less than 6, the flow is laminar (where \(Re = v \delta_f/v\); \(\delta_f\) is the fluid thickness; \(v\) is the kinematic fluid viscosity) and eq. (1) can be simplified and solved analytically if the penetration of oxygen into the fluid is assumed to be confined to a small region immediately below the air-liquid interface. This simplification, known as the penetration theory, was proposed by Hibbie and has been successfully applied to many chemical and environmental engineering problems, particularly in the field of air stripping.

A discussion of the penetration theory can be found in many introductory texts on mass transfer, and only a brief review is presented in this communication. In the region of oxygen penetration, the velocity of liquid is assumed constant and equal to the maximum fluid velocity \(v_{\text{max}}\). Solving eq. (1) for \(C(x,z)\) with these assumptions and with boundary conditions \(C = C^*\) at \(x = 0\) and \(C = 0\) as \(x\) approaches infinity, results in the steady state solution of

\[
\frac{C(x,z) - C_b}{C^* - C_b} = \text{erfc} \frac{x}{(4Dz/v_{\text{max}})^{1/2}} \tag{2}
\]

where \(C^*\) is the concentration of oxygen at the fluid surface in equilibrium with air; \(C_b\) is the initial and uniform concentration of oxygen in the entering fluid; \(x\) is the distance from the air-liquid surface; and \(z\) is the distance travelled by the fluid from the entrance.

Two factors that could affect the use of penetration theory for modelling oxygen transfer to fluids on biofilms are entrance effects and surface roughness, since these factors might induce turbulence in the flow. Considerable research has been done on entrance regions of laminar fluids over inclined surfaces. According to calculations by Stucheli and Ozisik, undisturbed laminar flow is developed within an entrance length of \(L_{\text{ent}}\), given by

\[
L_{\text{ent}} = 0.3 \frac{Re}{\delta_f} \tag{3}
\]

where \(\delta_f\) is the fluid thickness of the fluid under fully developed laminar flow conditions. Since Reynolds numbers for laminar flows are less than 6, entrance effects should be restricted to within two fluid thicknesses along the flow path. For laminar flow, surface roughness should not affect the flow profile. It is generally accepted that viscous effects at low Reynolds numbers damp out flow irregularities caused by surface
protrusions. This assumption concerning biofilm roughness would not be true for turbulent flow conditions as shown by Picologlou and co-workers and Siegrist and Gujer. Fully turbulent flow is not expected to occur for fluid flowing over flat plates below Reynolds numbers of ca. 250.

For the above conditions and assumptions, it is proposed that penetration theory [eq. (2)] be used to model oxygen transfer from the air to the fluid flowing over a biofilm. An example of an oxygen profile using this theory is shown in Figure 1 with the values assumed by Benefield and Molz of: $C^* = 8.0 \text{ mg/L}; C_b = 2 \text{ mg/L}; D = 1.15 \times 10^{-5} \text{ cm}^2/\text{s};$ a plate length and fluid depth of 100 and 10 cm, respectively; and a maximum fluid velocity that is 1.5 times the average fluid velocity, or $v_{\text{max}} = 0.0056 \text{ cm/s}$. The Reynolds number of this flow is less than 4 which indicates laminar flow conditions for the inclined plate model of Benefield and Molz. Figure 1 shows that as fluid moves along the plate, oxygen from the air does not diffuse deeper than ca. 1.5–2.0 cm before the fluid leaves the plate at a distance of 100 cm. Only the top 3 cm of fluid is shown in Figure 1 to enlarge the zone of oxygen penetration.

**OXYGEN TRANSFER TO THE BIOFILM**

As oxygen is consumed by microorganisms, an oxygen gradient will develop in the fluid immediately above the biofilm. The thickness of this oxygen gradient, or the mass transfer boundary layer, is a function of fluid motion and reaction rate in the biofilm. Williamson and McCarty have discussed the effect of fluid velocity on observed mass transfer rates. If the mass transfer boundary layer at the biofilm surface does not extend deeply enough into the fluid to reach the oxygen diffusing into the fluid from the air–liquid interface, then oxygen from the air–liquid interface will be unavailable to the biofilm. Since the oxygen flux is easily obtained from penetration theory, oxygen transfer to the biofilm could be uncoupled from a model of oxygen transfer to the biofilm, thus reducing the calculations necessary for a numerical model and avoiding the possibility of an oxygen flux to the biofilm caused by numerical dispersion.

To examine if oxygen penetration is insufficient to reach the biofilm, the relative thicknesses at steady state of the air–liquid and liquid–biofilm oxygen boun-

![Figure 1](image_url)  
*Figure 1.* Dissolved oxygen concentration in the fluid calculated using penetration theory [eq. (2)]. Only the top 3 cm of fluid is shown.
Boundary layers were compared using eq. (1) assuming laminar flow conditions, and the parameters previously specified. Two boundary conditions were required. As previously assumed for the penetration theory, the first boundary condition used was $C = C^*$ at $x = 0$. In the presence of a biofilm, the second boundary condition is normally that the oxygen flux at the biofilm is equal to the rate of oxygen removal ($R$) by the microorganisms in the biofilm, or $D \frac{dc}{dz} = R$ at $x = \delta_f$. However, a determination of the rate of the reaction is necessary for this boundary condition. Therefore, a limiting case of instantaneous reaction of oxygen at the biofilm surface was used which resulted in a maximum boundary layer thickness in the fluid above the biofilm. This second boundary condition for instantaneous reaction is $C = 0$ at $x = \delta_f$. The use of any other kinetics to describe oxygen transfer to the biofilm would result in a smaller uptake rate and therefore a decreased boundary layer thickness in the fluid above the biofilm.

The solution of eq. (1) with these two boundary conditions was obtained with a finite difference method employing a $51 \times 51$-node grid to obtain a two-dimensional oxygen profile within the fluid. Fluid velocities were estimated by assuming a parabolic velocity profile of laminar flow. The results at steady state shown in Figure 2 indicate that oxygen penetration is insufficient to reach either the biofilm or the boundary layer above the biofilm. In Figure 3, the oxygen profile at the plate exit is compared with the results of penetration theory near the fluid surface. As Figure 3 indicates, the finite difference method results in dissolved oxygen concentrations near the air–liquid interface that are not appreciably different from the results obtained using penetration theory. Furthermore, the maximum thickness of the oxygen boundary layer at the plate exit is ca. 3 cm for these flow conditions. Since the air–liquid and liquid–biofilm boundary layers are separated by a distance of at least 5 cm, oxygen diffusing from the air into the liquid can not reach the biofilm. Even the instantaneous disappearance of oxygen at the biofilm surface, which yields the maximum thickness of the boundary layer, does not influence an oxygen flux predicted by penetration theory for a 10-cm fluid thickness.

![Graph](image-url)

**Figure 2.** Dissolved oxygen concentration in the fluid assuming instantaneous removal of oxygen at the biofilm surface [eq. (1)].
An example of the errors involved in estimating the surface oxygen flux in the presence and absence of oxygen diffusion from the surface is provided using the results of Benefield and Molz. The overall oxygen flux to the biofilm surface, \( \Phi_{\text{total}} \), is:

\[
\Phi_{\text{total}} = D \left( \frac{C_{\text{at} \rightarrow \delta_b} - C_{\text{at} \rightarrow \delta_{\text{mr}}}}{\delta_{\text{mr}}} \right) \approx 0.9 \text{ mg/cm}^2 \text{ day} \quad (5)
\]

where the thickness of the liquid–biofilm layer is an input parameter defined to be \( \delta_{\text{mr}} = 0.001 \text{ cm} \). The advective flux is:

\[
\Phi_{\text{adv}} = \delta_N \frac{\partial C}{\partial z} = 0.3 \text{ mg/cm}^2 \text{ day} \quad (6)
\]

and the surface oxygen flux is estimated to be

\[
\Phi_{\text{surface}} = K_{\text{OL}} \frac{(C^* - C)}{\delta_b} \approx 0.6 \text{ mg/cm}^2 \text{ day} \quad (7)
\]

As expected, a mass balance shows the sum of the advective flux and the diffusive flux to be equal to the total flux of oxygen to the biofilm. A comparison of the advective flux to the total flux demonstrates that in this case approximately two thirds of the oxygen flux to the biofilm originates from the oxygen flux at the air–liquid surface. The analysis based on the penetration theory, however, shows that the surface flux of oxygen would be unavailable to the biofilm. Therefore the model of Benefield and Molz overestimates oxygen transfer to the biofilm in this example by 200%.

**DISCUSSION**

A biofilm model based on a completely vertically mixed fluid element for a 10-cm-thick fluid flowing over a biofilm at 322 cm/day results in an overestimation of the oxygen transfer from air to the biofilm. Assuming fluid is introduced over a biofilm surface at \( z = 0 \), for the flow conditions defined by Benefield and Molz, the penetration theory predicted that oxygen diffusing into the fluid would not extend through the fluid film to the biofilm surface. A vertically mixed fluid element would be appropriate only if fluid turbulence was induced by a mixing device or if the fluid was disturbed sufficiently to cause bulk fluid mixing. Disturbances in flow caused by entrance effects at \( \text{Re} < 4 \) could extend to a horizontal length of ca. 11 cm, but due to the low Reynolds number would probably be insufficient to cause substantial vertical mixing. If fluid is assumed mixed in the vertical direction, some degree of mixing in the horizontal direction in the model of Benefield and Molz should also be included.

For the flow conditions assumed by Benefield and Molz, it is suggested that their model of oxygen transfer within the fluid layer would be more realistic if laminar flow conditions were assumed and if the sur-
face oxygen term were deleted from eq. (4), resulting in:

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial z} - \frac{D}{\delta_b} \frac{\partial C}{\partial x} \bigg|_{x=\delta_b}$$  

(8)

The oxygen transfer from the air to the fluid can be calculated independently from calculations using eq. (8) using penetration theory [eq. (2)]. The oxygen utilized by the biofilm could be more accurately determined in a two-dimensional model using eq. (1) and the appropriate biofilm kinetics for the boundary condition at the liquid–biofilm interface. Unlike the model of Benefield and Molz, which requires the input of a thickness of the boundary layer above the biofilm, in a two-dimensional model this thickness would be fixed by the flow conditions and biofilm kinetics. Ordinarily, a two-dimensional numerical model must consider oxygen transfer throughout the fluid layer. However, since the oxygen diffusing from the air through the thick fluid film will not reach the biofilm, only the fluid near the biofilm needs to be modelled. For the physical conditions assumed in the above analysis, this means only the 3 cm fluid must be modelled versus 10 cm fluid. This reduction in fluid depth translates either to a savings in computational effort or to a greater resolution of the boundary layer at the biofilm surface for an equivalent number of calculations.

CONCLUSIONS

If oxygen transfer to biofilms is modelled under conditions for which the penetration theory is valid, only oxygen initially present in the liquid is available for aerobic reactions in the biofilm. It is suggested that the model of Benefield and Molz would be more generally useful if the oxygen transfer from air to bulk liquid was omitted and laminar flow conditions, rather than completely mixed flow conditions, were assumed. For short exposure times, oxygen diffusing into the liquid could only be made available to biofilms through fluid disruptions sufficient to cause vertical fluid mixing.

References