Oxygen penetration around burrows and roots in aquatic sediments

by F. J. R. Meysman1,2, O. S. Galaktionov2, R. N. Glud3 and J. J. Middelburg2,4

ABSTRACT

Diffusion is the dominant physical mechanism for the transfer of oxygen into fine-grained aquatic sediments. This diffusive uptake occurs at the sediment-water interface, but also at internal interfaces, such as along ventilated burrows or O2 releasing plant roots. Here, we present a systematic model analysis of the oxygen transfer at such biological interfaces. We list the equations for the O2 distribution, the flux, the oxygen penetration distance (OPD), the oxygenated sediment volume, and the irrigational oxygen uptake (IOU) as a function of biological parameters, such as burrow/root radius and burrow/root density. We also provide a set of computational “recipes” indicating how these model expressions can be used in the analysis of experimental data. As an example application, we show that the observed OPD reduction around ventilated burrows is largely due to the geometric effect of interface curvature. Because of this curvature effect, root and burrow surfaces cannot be treated as simple extensions of the sediment-water interface. As a general rule of a thumb, the burrow or root radius must be larger than OPD at the sediment-water interface to safely neglect geometrical corrections. Burrow and root systems in coastal environments typically do not meet this criterion.

1. Introduction

Oxygen plays a key role in the geochemistry, microbial ecology, and benthic biology of aquatic sediments (Canfield et al., 2005; Burdige, 2006; Glud, 2008). Accordingly, a common research objective in these disciplines is to unravel the mechanisms that govern the distribution and consumption of O2 within the sediment environment. A crucial quantity in this respect is the Total Oxygen Uptake (TOU) of the sediment, also known as the Sedimentary Oxygen Demand (SOD), which is typically quantified by enclosing a suitable sediment area and measuring the disappearance rate of O2 in the overlying water of this enclosure (e.g. Smith et al., 1997; Glud et al., 2003). The TOU is important because it serves as a proxy for the mineralization rate of organic matter, which is driving the benthic
ecosystem (Thamdrup, 2000; Glud, 2008). Yet, by its very nature, the TOU enclosure method adopts a black-box approach to oxygen consumption. Parameter sensitivity tests show that closed sediment incubations only provide marginal information on the spatial distribution of processes within the sediment (Andersson et al., 2006). Accordingly, TOU data \textit{an sich} do not reveal where the oxygen is consumed and how it is distributed within the sediment.

To better understand the factors controlling sedimentary oxygen consumption, TOU measurements have been complemented with data on $O_2$ distributions within the sediment. Such data collection was initiated by the development of oxygen micro-electrodes (Revsbech et al., 1980; Revsbech, 1989), and more recently stimulated by the advent of planar oxygen optode systems (Glud et al., 1996). These techniques have documented different zones of oxygen consumption within sediments (Brune et al., 2000): a shallow zone of oxygen penetration at the sediment-water interface (Revsbech et al., 1980; Rasmussen and Jørgensen, 1992), oxygenated shafts surrounding macrofaunal burrows (Jørgensen and Revsbech, 1985; Fenchel, 1996; Nielsen et al., 2004), and oxic microniches near the roots of seagrasses (Jensen et al., 2005; Frederiksen and Glud, 2006), saltmarsh plants (Sundby et al., 2003) and freshwater submerged macrophytes (Sand-Jensen et al., 1982; Laskov et al., 2006).

When making sedimentary oxygen budgets, the TOU is classically decomposed as a sum of independent contributions (the validity of this idealization is discussed below). In studies on macrofaunal irrigation, one typically uses the decomposition $\text{TOU} = \text{DOU} + \text{FR} + \text{IOU}$, which considers the Diffusive Oxygen Uptake (DOU) across the sediment-water interface, the faunal respiration (FR), and the Irrigational Oxygen Uptake (IOU) representing the $O_2$ consumption in the oxygenated zone around burrow (Archer and Devol, 1992; Wenzhofer and Glud, 2004). Similarly, in studies on vegetated sediments, one uses an analogous decomposition of the TOU, albeit with different terminology (e.g. Beckett et al., 2001; Frederiksen and Glud, 2006). Here, the TOU obtained from enclosed incubations in the dark is split as $\text{TOU} = \text{DOU} + \text{PR} + \text{ROL}$, which now features the plant respiration (PR) and the Radial Oxygen Loss (ROL). Historically, the IOU and ROL terms have originated from different fields, but conceptually, they are equivalent. For brevity, we will use the term IOU to refer to the oxygen uptake around both burrows and roots. Moreover, it is useful to introduce the “true” Sediment Oxygen Uptake (SOU), defined as $\text{SOU} = \text{DOU} + \text{IOU}$. The SOU specifies the geochemical/microbial consumption occurring within the “internal” sediment matrix, and thus excludes the respiration of plants and animals (which are considered “external” to the sediment).

The SOU thus consists of two terms (DOU and IOU) that are associated with two distinct zones of oxygenation (surface layer and deeper microniches). In marine environments, the individual contributions of these two terms depend on the distance from shore (Archer and Devol, 1992; Soetaert et al., 1996; Meile and Van Cappellen, 2003; Glud, 2008). In deep-sea sediments, the DOU provides the dominant contribution to the TOU (and hence the SOU). However, in nearshore environments and freshwater sediments, the contribution of the IOU
can be substantial: IOU values up to 80% of the TOU have been reported in bio-irrigated sediments (Wenzhofer and Glud, 2004) and up to 15% in seagrass beds (Jensen et al., 2005; Frederiksen and Glud, 2006). Accordingly, in coastal and shelf sediments, the IOU forms a controlling factor in the degradation of organic matter (Aller and Aller, 1998; Kristensen, 2000), and hence, it is necessary to gain a better understanding of the factors controlling the IOU.

There is, however, a strong asymmetry in our understanding of the DOU versus the IOU, both in terms of measurements and modeling. One reason for this is that the access to microzones around burrows and roots is rather difficult, while the sediment-water interface (SWI) is readily accessible to experimentation. Over the last two decades, oxygen dynamics near the SWI has been intensively studied, establishing mechanistic links between the DOU and \( \text{O}_2 \) profiles in the benthic boundary layer (Rasmussen and Jorgensen, 1992). Various controls on DOU variability have been examined, such as the influence of boundary layers (Jorgensen and Revsbech, 1985; Hondzo et al., 2005; Glud et al., 2007), microscale sediment topography (Roy et al., 2005), depth dependence of the volume-specific \( \text{O}_2 \) consumption rate (Epping and Helder, 1997; Berg et al., 1998), and nonsteady state boundary conditions (Higashino et al., 2004; Katsev et al., 2006).

In comparison, few studies have examined the connection between the IOU and the associated \( \text{O}_2 \) distributions around burrows and roots. Consequently, the IOU has remained much more a black box concept than the DOU. For example, detailed investigations of the SWI (Jorgensen and Marais, 1990; Roy et al., 2002, 2005) have revealed that in coastal sediments micro-topography explains up to 10% of the variability in the DOU. Yet, we are far from a comparable understanding of how factors such as burrow geometry and population density influence the IOU, which as noted above, accounts on average for 50% of the TOU in coastal, bio-irrigated sediments (Glud, 2008). The black box character of the IOU is illustrated by the fact that it is usually calculated indirectly, i.e., by the difference \( \text{IOU} = \text{TOU} - \text{DOU} - \text{FR} \) (Archer and Devol, 1992; Wenzhofer and Glud, 2004). Nonetheless, in recent years, a growing number of studies have reported \( \text{O}_2 \) distributions around roots (e.g Jensen et al., 2005; Frederiksen and Glud, 2006) and burrows (e.g Wang et al., 2001; Stief et al., 2004; Zorn et al., 2006) in coastal environments. So given these data, it should be possible to establish a direct mechanistic link between the IOU and the parameters of the oxygenated microniches that generate the IOU. To make this link in a truly quantitative way, one needs suitable mathematical models to analyze the data generated by micro-electrodes and planar optodes.

A number of pioneering modeling studies have examined the oxygenated zones around burrows (Aller, 1988; Fenchel, 1996) and roots (Armstrong, 1970). However, the results are scattered over the literature, and the theoretical development is partially incomplete. In this study, we summarize the necessary mathematical expressions in a systematic manner. This results in a single modeling framework that allows comparisons between different geometries of oxygenated microniches. Subsequently we test the validity of the resulting expressions against published and newly collected experimental data. Finally, we investigate
the factors controlling the oxygen penetration distance (OPD) around roots and burrows. An observation from past studies is that within the same sediment, the OPD around burrows or roots tends to be smaller than the OPD at the SWI. Various mechanisms have been proposed for this phenomenon, and our analysis will enable us to quantify the contribution of the mechanisms proposed.

2. Model development
   a. Modeling approach

   Oxic microniches within the sediment are created by biological structures that act as localized sources of oxygen (Brune et al., 2000; Glud, 2008). One type is due to macrofaunal burrows that are flushed with oxygenated water from the overlying water column (Aller, 2001; Koretsky et al., 2002). Oxygen diffuses through the burrow walls, which gives rise to a halo of oxic sediment around the burrow structure (Wenzhofer and Glud, 2004). A second type of oxic microniches stems from oxygen release in the rhizosphere of vascular plants (Sand-Jensen et al., 1982; Caffrey and Kemp, 1991). In salt marshes or seagrass meadows, oxygen is transported in the aerenchym of the plant roots, and then predominantly diffuses from the root tips (Sundby et al., 2003; Jensen et al., 2005; Frederiksen and Glud, 2006). From a modeling point of view, the oxygen release by these different biological structures (burrows and roots) can be captured by the same mechanism: they create a curved interface, from which oxygen diffuses deeper into the surrounding sediment, where the oxygen is finally consumed.

   The modeling of the O2 distribution along curved interfaces has a long history in biological research, dating back to the seminal work of Krogh (1919), who modeled the oxygen transfer from veins and arteries to the surrounding tissue. Mathematically, the resulting problem is referred to as a free-boundary problem, because the extent of the oxygenated zone needs to be determined as part of the solution; see Boudreau (2000) for a discussion of such free-boundary problems in the context of sediment biogeochemistry. Here, we will analyze the O2 free-boundary problem for three different model geometries that represent idealizations of sedimentary interfaces (Fig. 1). (1) Planar geometry - the sediment-water interface idealized as a perfectly flat surface. (2) Cylindrical geometry - a steadily and continuously ventilated burrow. (3) Spherical geometry - the root tip of a vascular plant approximated as a perfect sphere. Despite the difference in physical geometry, these three problems are one-dimensional from a mathematical point of view. Because of symmetry, the resulting equations will depend only on one spatial coordinate r, which either represents the distance from the planar interface (Fig. 1a), the radial distance from the symmetry axis of the cylinder (Fig. 1b), or the radial distance from the center of the sphere (Fig. 1c). The radius of the cylindrical burrow or spherical root tip is denoted as rs (the radius of the oxygen “source”). Note that our choice of a cylindrical geometry for burrows, and a spherical geometry for the oxygen release from apical region of roots primarily serves as an illustration on how to use the model equations. This choice, however, does not imply
generality. In fact, in some macrophytes oxygen is preferentially released from rhizomes (Caffrey and Kemp, 1991) or from the basal region of the roots rather than the tips (Laskov et al., 2006). In these cases, the cylindrical geometry would be more appropriate model, and the corresponding equations should be used.

b. Governing equation set

In all three cases, the steady-state distribution of oxygen near the interface is modelled by the mass balance equation

$$\phi D \nabla^2 c = R(c)$$

where $c$ is the oxygen concentration (expressed per unit volume of pore water), $\phi$ is the porosity, $D$ is the effective diffusion coefficient, and $R(c)$ denotes the oxygen consumption rate (expressed per unit volume of bulk sediment). The Laplace operator $\nabla^2$ originates from taking the divergence of the oxygen flux, and its specific form depends on the model geometry (planar $\nabla^2 = \frac{\partial^2}{\partial r^2}$; cylindrical $\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}$; spherical $\nabla^2 = \frac{2}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}$). At the interface between the sediment and the overlying water ($r = 0$) or at the the interface between the sediment and the burrow or root ($r = r_s$) the concentration is fixed at the constant value $c_0$. At the outer limit of the oxic zone ($r = r_0$), both the oxygen concentration and the flux (hence the gradient $\nabla c$) should vanish. This leads to the boundary conditions

$$c|_{r=r_s} = c_0, \quad c|_{r=r_0} = 0, \quad \nabla c|_{r=r_0} = 0.$$
Table 1. List of mathematical symbols with their dimensions. [L] stands for units of length, [T] units of time, and [A] units of mass (for example “mol” in SI). For reference, SI units are listed explicitly.

The concentration $c_0$ is expressed per unit volume of pore water.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Variable</th>
<th>Dimensions</th>
<th>SI units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
<td>[L]$^2$[T]$^{-1}$</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$c_0$</td>
<td>Concentration at the interface</td>
<td>[A][L]$^{-3}$</td>
<td>mol m$^{-3}$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Sediment porosity</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$R_0$</td>
<td>Oxygen consumption rate</td>
<td>[A][L]$^{-3}$[T]$^{-1}$</td>
<td>mol m$^{-3}$ s$^{-1}$</td>
</tr>
<tr>
<td>$F$</td>
<td>Flux at the interface</td>
<td>[A][L]$^{-2}$[T]$^{-1}$</td>
<td>mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$r$</td>
<td>Spatial coordinate</td>
<td>[L]</td>
<td>m</td>
</tr>
<tr>
<td>$r_s$</td>
<td>Radius of the root or burrow</td>
<td>[L]</td>
<td>m</td>
</tr>
<tr>
<td>$r_0$</td>
<td>Location where oxygen vanishes</td>
<td>[L]</td>
<td>m</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Oxygen penetration distance</td>
<td>[L]</td>
<td>m</td>
</tr>
</tbody>
</table>

Note that the location where oxygen disappears $r_0$ must be determined as part of the solution. The extent of the oxic zone is then given by the oxygen penetration distance (OPD), defined as $\delta = r_0 - r_s$. Table 1 provides an overview of all model parameters together with their units.

The model adopted here incorporates some important simplifications, which are justifiable in a first-order approximation. First of all, the model assumes steady state, which is not necessarily satisfied under natural conditions. Burrow ventilation can lead to oscillating O$_2$ concentrations within the burrow (Boudreau and Marinelli, 1994), while also the oxygen consumption around roots shows its own temporal dynamics. Secondly, the porosity and diffusion coefficient are assumed constant throughout the zone of oxygen consumption. However, it has shown that burrow linings can modify diffusivity and/or porosity near burrow walls (Aller, 1983; Hannides et al., 2005), while iron plaques can modify the diffusion around roots (Moller and Sand-Jensen, 2008). This issue is further discussed below. Thirdly, the oxygen consumption rate is taken constant throughout the oxic zone, and vanishes elsewhere

$$R(c) = \begin{cases} R_0, & c > 0 \\ 0, & c = 0 \end{cases}$$

(3)

where the oxygen consumption rate $R_0$ is expressed per unit of bulk sediment. This simple parametrization is frequently used in studies on O$_2$ dynamics in aquatic sediments (Revsbech et al., 1980; Cai and Sayles, 1996), because it successfully reproduces observations. Moreover, it enables a simple analytical solution to the mass balance (1), which greatly facilitates the sensitivity analysis of the resulting model expressions. The above kinetic rate law incorporates two idealizations when compared to other rate expressions. Firstly, it does not have the saturation effect at low O$_2$ levels as in the traditional Monod expression $R(c) = R_0c/(c + K_S)$, where $K_S$ is the half-saturation constant (Rabouille and Gaillard, 1991). Although the Monod rate law provides a more realistic representation of microbial
substrate uptake, its nonlinearity necessitates a numerical solution (requiring dedicated software, which can be time consuming). Moreover, the half saturation constant for oxygen uptake in sediments is typically low (i.e. < 5 μmol L⁻¹), and lies close to the detection limit of the experimental methods. Accordingly, the Monod rate will behave similarly as the simplified expression above. A second, and less straightforward, idealization embedded in the rate expression (3) is that the $R_0$ value is assumed constant throughout the oxygenated zone. In some coastal sediments, this appears to be a reasonable assumption (Rasmussen and Jorgensen, 1992; Higashino et al., 2004). On other occasions, a clear increase of the oxygen consumption rate is observed near the oxic-anoxic interface due to re-oxidation of reduced products from anoxic mineralization transported upwards (Soetaert et al., 1996; Berg et al., 1998). Similarly, investigation of O₂ profiles near burrows indicates that the oxygen consumption rate is not always spatially homogeneous (Nielsen et al., 2004). Burrow walls can act as hot-spots of microbial activity, while O₂ consumption can increase due to lateral diffusion of reduced components towards the burrow (see discussion in connection to Fig. 4 below). Similar considerations apply to root systems, where intravascular O₂ concentrations are changing, and plant roots excrete DOC, which may locally enhance the O₂ consumption (Beckett et al., 2001). Still, all this complexity observed under natural conditions does not mean that the idealized assumptions employed here are without value. As shown below, we will use the simplified model (3) as a starting point to explore the dominant controls on the oxygen penetration distances and oxygenated volumes in sediments. Nonetheless, when applying the model solutions to actual data, the simplifying assumptions should be kept in mind and critically evaluated.

3. Recipes for model application

The analytical solutions for the O₂ free boundary problem in the planar, cylindrical and spherical geometries (Fig. 1) can be obtained by standards methods of differential calculus. The expressions for the oxygen penetration distance, the oxygen profile and the resulting oxygen flux at the interface are summarized in Table 2. In this section, we will detail how these expressions can be applied to experimental data. Effectively, we will present a set of computational “recipes,” which correspond to actual data collection procedures.

a. The O₂ profile from a known oxygen consumption rate

The model solutions for the three geometries require the specification of the same set of five parameters: the effective diffusion coefficient $D$, the oxygen concentration at the interface $c_0$, the porosity $\phi$, the source radius $r_s$, and the oxygen consumption rate $R_0$. Note that these parameters should be specified at the exact location where they are applied (i.e. the sediment water interface, the sediment surrounding the burrow, or the root tip). In a first type of application, we assume that suitable values for each of these parameters are available. Estimates for the parameters $\phi$, $c_0$, and $r_s$ are relatively easy to determine experimentally. Furthermore, the effective diffusion coefficient $D$ may be obtained by first
Table 2. Expressions for the oxygen penetration distance $\delta$ and the concentration profile $c$ based on a known oxygen consumption rate $R_0$ or a known flux $F$. The expressions for the concentration profile $c$ are valid in the interval $r_s < r < r_s + \delta$, where $r_s$ is the source radius. In the planar case, $r_s = 0$ so that this interval becomes $0 < r < \delta$. The three solutions for the OPD in the spherical case are respectively valid in the ranges $0 < r_s < \sqrt{3}\lambda$, $r_s = \sqrt{3}\lambda$, and $r_s \geq \sqrt{3}\lambda$. One can prove that in the spherical geometry, the length scale $\xi$ is always constrained by $\xi < 2r_s$ for any finite OPD.

<table>
<thead>
<tr>
<th></th>
<th>RATE BASED</th>
<th>FLUX BASED</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length scale</td>
<td>$\lambda = \sqrt{\frac{2\phi Dc_0}{R_0}}$</td>
<td>$\xi = \frac{2\phi Dc_0}{F}$</td>
</tr>
<tr>
<td>PLANAR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OPD</td>
<td>$\delta = \lambda$</td>
<td>$\delta = \xi$</td>
</tr>
<tr>
<td>Profile</td>
<td>$c = \frac{c_0}{\lambda^2} (\delta - r)^2$</td>
<td>$c = \frac{c_0}{\xi^2} (\delta - r)^2$</td>
</tr>
<tr>
<td>Flux/Rate</td>
<td>$F = R_0 \delta$</td>
<td>$R_0 = \frac{F}{\delta}$</td>
</tr>
<tr>
<td>CYLINDRICAL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OPD</td>
<td>$r_s \delta + \frac{\delta^2}{2} - (r_s + \delta)^2 \ln \frac{r_s + \delta}{r_s} + \lambda^2 = 0$</td>
<td>$(\delta + \frac{\delta^2}{2r_s}) (r_s + \xi)$</td>
</tr>
<tr>
<td>Profile</td>
<td>$c = \frac{c_0}{\lambda^2} \left[ \frac{r_s^2}{2} - (r_s + \delta)^2 \left( \frac{1}{2} + \ln \frac{r_s}{r_s + \delta} \right) \right]$</td>
<td>$c = \frac{c_0}{\xi^2} \left( 1 + \frac{\delta}{2r_s} \right)^{-1}$</td>
</tr>
<tr>
<td>Flux/Rate</td>
<td>$F = R_0 \delta \left( 1 + \frac{\delta}{2r_s} \right)$</td>
<td>$R_0 = \frac{F}{\delta} \left( 1 + \frac{\delta}{2r_s} \right)^{-1}$</td>
</tr>
<tr>
<td>SPHERICAL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OPD</td>
<td>$\delta = \left{ \begin{array}{cc} r_s \cosh \left( \frac{1}{3} \arccosh \frac{6\lambda^2 - r_s^2}{r_s^2} \right) - \frac{r_s}{2} \ \frac{r_s \cos \left( \frac{1}{3} \arccos \frac{6\lambda^2 - r_s^2}{r_s^2} \right)}{3} - \frac{r_s}{2} \end{array} \right}$</td>
<td>$\delta = r_s \frac{3\xi - 3r_s + \sqrt{3}(r_s + \xi)(3r_s - \xi)}{4r_s - 2\xi}$</td>
</tr>
<tr>
<td>Profile</td>
<td>$c = \frac{c_0}{\lambda^2} \left[ \frac{r_s^2}{3} + \frac{2(r_s + \delta)^3}{3r_s} - (r_s + \delta)^2 \right]$</td>
<td>$c = \frac{c_0}{\xi^2} \left( 1 + \frac{\delta}{r_s} + \frac{\delta^2}{3r_s^2} \right)^{-1}$</td>
</tr>
<tr>
<td>Flux/Rate</td>
<td>$F = R_0 \delta \left( 1 + \frac{\delta}{r_s} + \frac{\delta^2}{3r_s^2} \right)$</td>
<td>$R_0 = \frac{F}{\delta} \left( 1 + \frac{\delta}{r_s} + \frac{\delta^2}{3r_s^2} \right)^{-1}$</td>
</tr>
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</table>

Calculating the molecular diffusion coefficient at a specific temperature and salinity using the relations given in Boudreau (1997), and subsequently using an appropriate tortuosity correction (Boudreau, 1996; Boudreau and Meysman, 2006). The oxygen consumption rate $R_0$ is more difficult to measure accurately, but an indicative (potential) value can be estimated from sediment slurry incubations (e.g. Dauwe et al., 2001; Frederiksen and Glud, 2006).

If the values for these five parameters are known, one can employ the solutions directly as listed in the first column of Table 2. Their application consists of three steps. The first step is to compute the characteristic length scale $\lambda$ as
This length scale has the same units as the spatial coordinate $r$, and suitably combines all geochemical parameters that influence the local $O_2$ distribution. Mathematically, the length scale results from bringing the $O_2$ free boundary problem into a non-dimensional form. Physically, one could say that it specifies the “geochemical climate” near a given interface.

In a second step, one can use the length scale $\lambda$ to determine the oxygen penetration distance $\delta$. In the planar case, this is straightforward: $\delta$ simply equals the length scale $\lambda$. In the spherical case, one obtains a cubic equation, which has a direct analytical solution (Table 2). In the cylindrical case, the determination of the OPD is slightly more involved: $\delta$ should be numerically solved from a transcendent equation (Table 2). This can be done by root solving routines in standard math packages (e.g., R, excel, matlab). Once the oxygen penetration distance $\delta$ is known, one can proceed to the third step: the associated oxygen concentration profile $c(r)$ and the associated flux across the interface $F$ can be calculated.

### b. The $O_2$ profile from a known interface flux

In many situations, the value of the oxygen consumption rate $R_0$ is not known beforehand, but needs to be determined from the model. Instead, data on the flux $F$ can be available from whole core incubations. For example, in studies on bio-irrigation in muddy sediments (Wenzhofer and Glud, 2004), one can (1) determine the total oxygen uptake (TOU) from a closed sediment incubation incorporating fauna, (2) measure the diffusive oxygen uptake (DOU) in a control core where fauna has been removed or inhibited, (3) determine the faunal respiration (FR) from available empirical physiological relations and laboratory-determined respiration measurements (Banta et al., 1999), (4) calculate the irrigational oxygen uptake (IOU) as $IOU = TOU - DOU - FR$, and (5) determine the flux as $F = IOU/A_b$, where $A_b$ represents the total burrow surface area per unit area of sediment-water interface. Accordingly, we arrive at the situation where $\phi$, $c_0$, $D$ and $r_s$ are known as in the previous case, but where $F$ is specified instead of $R_0$. Accordingly, one cannot calculate the length scale $\lambda$ on which the model solutions are based.

To resolve this, one can restate the model solutions in terms of the interface flux $F$ as shown in the second column of Table 2. Again, the application of the expressions consists of three steps. First, one needs to compute a new characteristic length scale $\xi$, which is now defined in terms of the measured flux value

$$\xi = \frac{2\phi D c_0}{F}.$$  

After that, one needs to determine the oxygen penetration distance $\delta$. In the planar case, one simply obtains that $\delta = \xi$. In other words, the length scale $\xi$ is again the oxygen penetration distance that would be observed for a flat interface

$$\delta_{\text{planar}} = \lambda_{\text{planar}} = \xi_{\text{planar}}.$$
It is important to note that the above equality only holds for the planar case, and not for the cylindrical and spherical case. In the spherical case, the OPD is determined as the positive root of the quadratic equation (Table 2, second column). In the cylindrical case, the OPD is obtained by the numerical solution of a transcendent equation. Similar to the procedure in the previous section, the computed value of $\delta$ can be used to arrive at remaining unknowns, i.e., the concentration profile $c(r)$ and the oxygen consumption rate $R_0$.

c. Oxygenated sediment volume

The relations in Table 2 describe in detail the oxic zone around a single burrow or root. This knowledge can be upscaled to a “population” of burrows and roots to estimate the oxygenated volume and oxygen uptake on a per m$^{-2}$ basis assuming no overlaps of the oxic halo’s. This procedure then allows to investigate how biological parameters, such as burrow/root radius and burrow/root density, influence the oxygen uptake of sediments.

As noted in the introduction, part of the “true” sediment oxygen uptake is linked to diffusion across the SWI, and part is associated with the oxygenated zones around roots and burrows. An interaction between these two mechanisms occurs when roots or burrows intersect the oxic layer at the sediment surface. In near-shore sediments however, this zone of intersection is typically small, as oxygen vanishes rapidly at the surface (below a few millimeters). Roots and burrows typically penetrate much deeper (on the order of centimeters) into the anoxic zone (Aller, 2001; Koretsky et al., 2002). Ignoring this small interaction, one can idealize the total oxic volume as consisting of two independent parts: an oxic volume $V_{\text{ox}_1}^\text{swi}$ sustained by diffusive transport across the SWI, and an irrigated volume $V_{\text{ox}_2}^\text{irr}$ sustained by diffusion across biological interfaces

$$V_{\text{ox}} = V_{\text{ox}_1}^\text{swi} + V_{\text{ox}_2}^\text{irr}$$

Note that when the oxygenated volumes are expressed per unit area of SWI, they each represent an (apparent) depth layer of oxygenated sediment. For the SWI, this thickness simply equals the oxygen penetration depth. For the irrigated volume $V_{\text{ox}_2}^\text{irr}$, this becomes an imaginative layer in which all oxic zones around burrows or roots are merged together.

Burrows are often referred to as extensions of the sediment water interface. If not carefully interpreted, this metaphor could suggest that irrigated volume $V_{\text{ox}_2}^\text{irr}$ can be simply estimated by multiplication of the burrow interface area $A_{\text{int}}$ with the OPD at the SWI. However, this simple upscaling procedure is rarely justified, and to assess its accuracy, we can express the irrigated volume as

$$V_{\text{ox}_2}^\text{irr} = \gamma_{\text{int}} A_{\text{int}} \delta_{\text{swi}} \approx \gamma_{\text{int}} \left( \frac{A_{\text{int}}}{A_{\text{swi}}} \right) V_{\text{swi}}^\text{ox},$$

The factor $A_{\text{int}}/A_{\text{swi}}$ provides the surface area enlargement due to the presence of biological interfaces. The $\gamma_{\text{int}}$ factor quantifies the “error” introduced when using the simplistic surface area upscaling: it accounts for the fact that burrow interfaces are curved, and that local
Table 3. Expressions for the oxygenated volume per unit SWI area and the oxygen uptake in a sediment containing a population of burrows or roots. In these, \( n_b \) represents the burrow density per unit SWI area, \( r_b \) the burrow radius, \( L_b \) the average burrow length, \( A_b \) the total burrow surface area per unit SWI area, \( V_b \) the total burrow volume per unit SWI area, and \( R_b \) the oxygen consumption rate around the burrow. Similarly, \( n_r \) is the density of spherical root nodules per unit SWI area, \( r_r \) the root nodule radius, \( A_r \) the total root surface area per unit SWI area, \( V_r \) the total root volume per unit SWI area, and \( R_r \) the oxygen consumption rate near the root interface.

Surface layer

\[
V_{ox}^{swi} = \delta_{swi} \\
DOU = F_{swi} = R_{swi} \delta_{swi}
\]

Burrow zones

\[
A_b = n_b L_b 2 \pi r_b , \quad V_b = n_b L_b \pi r_b^2 \\
V_{int}^{ox} = n_b L_b \pi (r_0^2 - r_b^2) = V_b \frac{2}{r_b} \delta_b \left(1 + \frac{\delta_b}{2 r_b}\right) = A_b \delta_b \left(1 + \frac{\delta_b}{2 r_b}\right)
\]

\[
IOU = A_b F_b = A_b R_b \delta_b \left(1 + \frac{\delta_b}{2 r_b}\right)
\]

\[
\gamma_b = \frac{\delta_b}{\delta_{swi}} \left(1 + \frac{\delta_b}{2 r_b}\right)
\]

Root zones

\[
A_r = n_r 4 \pi r_r^2 , \quad V_r = n_r (4 \pi/3) r_r^3 \\
V_{int}^{ox} = n_r \frac{4 \pi}{3} (r_0^3 - r_r^3) = V_r \frac{3}{r_r} \delta_r \left(1 + \frac{\delta_r}{r_r} + \frac{\delta_r^2}{3 r_r^2}\right) = A_r \delta_r \left(1 + \frac{\delta_r}{r_r} + \frac{\delta_r^2}{3 r_r^2}\right)
\]

\[
IOU = A_r F_r = A_r R_r \delta_r \left(1 + \frac{\delta_r}{r_r} + \frac{\delta_r^2}{3 r_r^2}\right)
\]

\[
\gamma_r = \frac{\delta_r}{\delta_{swi}} \left(1 + \frac{\delta_r}{r_r} + \frac{\delta_r^2}{3 r_r^2}\right)
\]

d. Irrigational oxygen uptake

The two types of oxygenated zones are each linked to a specific type of oxygen uptake. As a result, the sediment oxygen uptake (SOU) can also be split into two independent parts: diffusive oxygen uptake (DOU) across the SWI, and the irrigational oxygen uptake (IOU) across biological interfaces

\[
SOU = DOU + IOU.
\]
A central assumption in our model is that the oxygen consumption rate remains constant within the oxygenated zone. Because of this, the two uptake rates must scale with the corresponding oxygenated volume

\[
\text{DOU} = R_{swi} V_{ox}^{swi} \tag{10}
\]

\[
\text{IOU} = R_{int} V_{ox}^{int} \tag{11}
\]

where \( R_{swi} \) and \( R_{int} \) are the respective oxygen consumption rates within the surface layer and near the biological interfaces. Note that only when the consumption rate near biological interfaces and near the SWI are similar (when \( R_{swi} = R_{int} = R_0 \)), one obtains a simple relation between the total consumption rate and total oxygenated volume in the sediment (\( SOU = R_0 V_{ox} \)). As was done for the irrigated volume, one can express the IOU in terms of properties at the sediment-water interface

\[
\text{IOU} = \gamma_{int} \left( \frac{R_{int}}{R_{swi}} \right) \left( \frac{A_{int}}{A_{swi}} \right) \text{DOU} \tag{12}
\]

Accordingly, the difference between IOU and DOU is governed by a combination of three factors: surface area increase (\( A_{int}/A_{swi} \)), a modulation of the oxygenated volume through curvature and local geochemical factors (\( \gamma_{int} \)), and differences in O\(_2\) reactivity (\( R_{int}/R_{swi} \)). The appropriate expressions for the IOU are again summarized in Table 3.

4. Results

a. Modeling oxygen profiles around burrows and roots

In recent years, micro-electrode and optode techniques have enabled high resolution data on O\(_2\) distributions around burrows and roots (e.g. Wang et al., 2001; Wenzhofer and Glud, 2004; Frederiksen and Glud, 2006). To analyze such data in a quantitative fashion, one can employ the mathematical expressions provided in Table 2. Yet, when applying these formulas in any practical situation, one is immediately confronted with following obstacle: the length scales \( \lambda \) and \( \xi \) should be calculated based on the parameter values near the curved interface. In many cases, one has no direct information about the oxygen consumption rate \( R_{int} \) nor the flux \( F_{int} \) near burrows and roots, and hence, one cannot use the procedures outlined above to predict the associated OPD and oxygen distribution \( c(r) \). This is because the necessary measurements near burrow and root interface are cumbersome, and vulnerable to disturbance and artifacts (e.g. the wall effects of planar O\(_2\) optodes prohibit direct estimation of fluxes; slurries provide an estimate of the bulk consumption rate, but not necessarily \( R_{int} \)). In a similar way, when the porosity \( \phi \) or the diffusivity \( D \) are measured in the bulk sediment, one does not know how representative these values are for the burrow/root interface. Barring such information, one cannot calculate the geochemical length scales \( \lambda_{int} \) and \( \xi_{int} \) at the biological interface.

Fortunately, there is a simple approximative procedure to still calculate oxygen distributions, provided that the OPD at the SWI is known (which is commonly the case). At the
Figure 2. Oxygen distributions near the burrow of the mayfly *Hexagonia limbata*: comparison of the model predicted profiles with micro-electrode data. Data obtained from Wang et al. (2001). (a) Oxygen profile at the sediment-water interface. The planar expression for the oxygen profile $c(r)$ is fitted to the data to extract the length scale $\lambda_{swi}$. (b) Oxygen profile in the sediment surrounding the burrow. The radial oxygen profile $c(r)$ near the burrow is predicted from the $\lambda_{swi}$ value obtained in (panel a). Hence, no fitting is used to obtain the model profile in (panel b).

SWI, the OPD simply matches the geochemical length scale ($\lambda_{swi} = \delta_{swi}$). We can take advantage of this, and express the geochemical length scale at the internal interfaces as

$$\lambda_{int} = \sqrt{\frac{c_{int}}{c_{swi}} \frac{\phi_{swi} D_{swi}}{\phi_{int} D_{int}} \frac{R_{swi}}{R_{int}} \frac{c_{int}}{c_{swi}} \delta_{swi}}.$$  \hspace{1cm} (13)

The subscripts $swi$ and $int$ respectively refer to values at the SWI and near the interface (burrow wall or root surface). In effect, Eq. (13) nicely identifies the different factors controlling the geochemical climate near burrows or roots: porosity and diffusivity differences ($\phi_{swi} D_{swi}/\phi_{int} D_{int}$), increased “hotspot” O$_2$ consumption ($R_{swi}/R_{int}$), and difference in burrow oxygenation ($c_{int}/c_{swi}$). Depending on the available data, one can make a suitable approximation of the unknown $\lambda_{int}$ by ignoring one or more of the square root factors. An analogous expression to (13) can be written for the length scale $\xi_{int}$.

We applied this procedure to micro-electrode oxygen profiles from a sediment containing burrows of the mayfly *Hexagenia limbata*, as presented in Wang et al. (2001). Figure 2 shows both the oxygen profile data recorded at the sediment-water interface and across the burrow. Using the known value $c_{swi} = 279 \mu$mol L$^{-1}$, the planar expression for the oxygen profile $c(r)$ (Table 2, RATE BASED/Planar/Profile) was fitted to the oxygen data using a least squares regression method (Fig. 2a), yielding an oxygen penetration $\delta_{swi} = 3.4$ mm. As a starting hypothesis, we assumed that differences in porosity, diffusivity, and consumption rate between the SWI and the burrow surroundings were negligible. As a result, Eq. 13 simplifies to

$$\lambda_{int} = \sqrt{\frac{c_{int}}{c_{swi}} \delta_{swi}}.$$  \hspace{1cm} (14)
Figure 3. Oxygen distributions near a silicone sphere embedded in homogenized sediment in a laboratory set-up: Comparison of the model predicted profiles with micro-electrode data. (a) Oxygen profile at the sediment-water interface. The planar expression for the oxygen profile \( c(r) \) is fitted to the data to extract the parameter \( \lambda_{swi} \). (b) Oxygen profile in the sediment surrounding the sphere. The radial oxygen profile \( c(r) \) near the sphere is predicted from the \( \lambda_{swi} \) value obtained in (panel a). Hence, no fitting is used to obtain the model profile in (panel b).

Implementing this equation with \( c_{int} = 259 \mu \text{mol L}^{-1} \), we obtained \( \lambda_{int} = 3.3 \text{ mm} \). Using this \( \lambda \)-value and the measured burrow radius \( r_s = 1.2 \text{ mm} \), we predict an OPD near the burrow \( \delta_b \) of 2.7 mm (Table 2, RATE BASED/Cylindrical/OPD). The predicted oxygen profile near the burrow (Table 2, RATE BASED/Cylindrical/Profile) is compared to the data in Figure 2b. Overall there is good agreement between the model prediction and the observed profile. Both at the sediment surface and near the burrow wall, the simulated oxygen profiles show a stronger curvature and somewhat deeper oxygen penetration than the measured profiles. This indicates that the average value of the consumption rate \( R_{int} \) is probably similar to that at the SWI, but that \( R_{int} \) might not be constant throughout the oxic zone. Reduced substances (e.g., NH4 or H2S resulting from organic matter diagenesis) diffuse towards the burrow, and are re-oxidized in a narrow zone around the OPD (Soetaert et al., 1996). Such natural heterogeneity in the oxygen consumption would straighten the oxygen profiles as observed in the data profile, but is not accounted for in our simplified model.

In a similar way, we also applied the above procedure to data within a spherical geometry. No micro-electrode data near actual root tips were available, and so, we made a laboratory set-up that mimics a spherical oxygen source. A silicone sphere of outer radius 0.95 mm was placed in a homogenized sediment, with a constant air supply to ensure a constant internal \( O_2 \) concentration within the sphere. The set-up was allowed to stand for three days to reach a steady state situation. Figure 3 shows the oxygen profiles recorded at the sediment-water interface and near the sphere. With \( c_{swi} = 156.2 \mu \text{mol L}^{-1} \), the planar expression for the oxygen profile \( c(r) \) (Table 2, row 3, column 1) was again fitted to the SWI data using a least squares regression method (Fig. 3a), now resulting in \( \delta_{swi} = 1.31 \text{ mm} \).
Implementing Eq. 14 with $c_{int} = 86.7 \, \mu\text{mol L}^{-1}$, we then obtained $\lambda_{int} = 0.98 \, \text{mm}$. Using this $\lambda$-value and $r_s = 0.95 \, \text{mm}$, the predicted OPD near the sphere was $\delta_s = 0.78 \, \text{mm}$ (Table 2, RATE BASED/Spherical/OPD). The predicted oxygen profile (Table 2, RATE BASED/Spherical/Profile) is in excellent agreement with the observed radial profile from the sphere (Fig. 3b). Consequently, differences in porosity, diffusivity, or consumption rate between interface and SWI seem negligible, as expected in this homogenized artificial set-up.

\section*{b. Factors controlling the OPD near burrows and roots}

In the planar case, the OPD simply matches the geochemical length scale $\lambda$ (or $\xi$). This way, the OPD at the SWI serves as a natural benchmark to compare the OPD along cylindrical and spherical surfaces within the same sediment. In the past, oxygen measurements have revealed marked differences between the OPD at the SWI and the OPD around burrows and roots within the same sediment (e.g. Fenchel, 1996; Zorn \textit{et al.}, 2006). To improve our understanding of bio-irrigated sediments, it is crucial to be able to explain these observed differences.

Suppose we have observed a certain OPD value $\delta_{int}^{\text{observed}}$ near an interface which is different from the observed value $\delta_{swi}^{\text{observed}}$ at the SWI. This difference can be caused by the curvature of the interface or local geochemical factors (like partial burrow oxygenation and increased O$_2$ consumption as indicated in Eq. 13). To systematically test what factors are dominant, we propose a procedure that generates a series of model estimates $\delta_{int}^{\text{model}}$, based on a model that is gradually made more complex. To start with, we can assume that curvature is the overriding effect. In other words, we can assume that the geochemical climate is exactly the same as at the SWI, and calculate the $\lambda_{int}^{C}$ value that would be observed if curvature would be the only effect playing. This is simply done by using the value of $\lambda_{swi}$ in the equations for $\delta_{int}$ in Table 2. Subsequently, we can add one or more effects of local geochemistry. To this end, we can modify the geochemical length scale at the interface, by incorporating one or more of the square root factors in expression (13). Using this “updated” value for $\lambda_{int}$, one can calculate a new “updated” estimate $\delta_{int}^{G+C}$, which now accounts for curvature (C) and geochemistry (G). The whole procedure can be summarized as

$$\delta_{int}^{\text{model}} = \left( \frac{\delta_{int}^{G+C}}{\delta_{swi}^{C}} \right) \left( \frac{\delta_{int}^{C}}{\delta_{int}^{G}} \right) \delta_{swi}$$

(15)

The factors between brackets factors respectively account for the effects of curvature and local geochemistry. Different models can be tested by incorporating different square root factors in expression (13). To check how much a given model explains of the observed difference between, one can introduce the ratio

$$\beta = \frac{\delta_{int}^{\text{model}} - \delta_{int}^{\text{observed}}}{\delta_{swi}^{\text{observed}} - \delta_{swi}^{\text{observed}}} \times 100\%.$$  

(16)
Table 4. Importance of curvature for oxygen penetration near the ventilated burrows. \( \delta_{swi} \) is the OPD at sediment-water interface, \( \delta_{b} \) is the OPD near the burrow wall. The relative contribution factors beta, as defined as in Eq. (16), accounts for geometry (\( \beta_{1} \)), partial oxygenation of burrows (\( \beta_{2} \)) and increased microbial respiration near the burrow-sediment interface (\( \beta_{3} \)). Experimental data for burrowing macrofauna are taken from (1) Fenchel (1996), (2) Wang et al. (2001), (3) Zorn et al. (2006), and (4) Stief et al. (2004). Only those species from Zorn et al. (2006) are included for which the sediment properties around the burrow are similar to those at the SWI. Fenchel (1996) provides no actual data on burrow O\(_2\) concentrations, but shows microprofiles taken at the sediment surface and inside the burrow 1 cm beneath the sediment surface. These profiles show similar concentrations at the burrow wall and SWI, and based on this, we assumed that the concentration at the burrow wall \( c_{int} \) is the same as the concentration \( c_{swi} \) at the SWI. This assumption is not representative for the whole Nereis burrow as deeper lying parts will show reduced oxygenation.

| Species                | (ref) | \( r_{s} \) | \( c_{int} / c_{swi} \) | \( \delta_{int} \) | \( \delta_{swi} \) | \( \delta_{b} \) | \( \delta_{1} \) | \( \beta_{1} \) | \( \delta_{2} \) | \( \beta_{2} \) | \( \delta_{3} \) | \( \beta_{3} \) | \( \text{MEAN} \) |
|------------------------|-------|--------------|--------------------------|---------------------|-----------------|-----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|---------|
| Nereis diversicolor    | (1)   | 0.55         | 1.0                      | 1.65                | 0.96            | 1.33            | 47%            | 1.33           | 0%             | 0.96           | 53%            | 18%            | 0%              | 50%     |
|                        |       | 0.9          | 1.0                      | 1.9                | 1.59            | 49%             | 1.59           | 0%             | 1.26           | 51%            | 12%            |                 | 50%     |
|                        |       | 0.75         | 1.0                      | 1.4                | 0.75            | 1.19            | 33%            | 1.19           | 0%             | 0.75           | 67%            | 26%            |                 | 50%     |
|                        |       | 0.6          | 1.0                      | 1.4                | 1.5             | 2.28            | 48%            | 2.28           | 0%             | 1.50           | 52%            | 23%            |                 | 50%     |
| Hexagenia limbata      | (2)   | 1.2          | 0.96                     | 2.5                | 2.09            | 81%             | 2.06           | 8%             | 2.00           | 11%            | 1%             |                 | 50%     |
| Sialis velata          |       | 2.2          | 0.82                     | 2.5                | 2.21            | 29%             | 2.02           | 19%            | 1.50           | 52%            | 16%            |                 | 50%     |
| Corophium volutator    | (3)   | 1.25         | 1.0                      | 2.6                | 2.2             | 106%            | 2.18           | 0%             | 2.20           | −6%            | −1%            |                 | 50%     |
| Heteromastus filiformis|       | 0.75         | 1.0                      | 0.6                | 0.55            | 54%             | 0.55           | 0%             | 0.50           | 46%            | 4%             |                 | 50%     |
| Arenicola marina       |       | 3.25         | 1.0                      | 1.1                | 0.95            | 34%             | 1.05           | 0%             | 0.95           | 66%            | 5%             |                 | 50%     |
| Ephoron virgo          | (4)   | 1.5          | 0.87                     | 4.1                | 2.0             | 33%             | 3.34           | 10%            | 2.00           | 54%            | 25%            |                 | 50%     |
|                        |       | 1.5          | 0.87                     | 2.6                | 1.5             | 2.22            | 35%            | 2.08           | 12%            | 1.50           | 53%            | 18%            |                 | 50%     |
| MEAN                   |       |              |                          | 50%                |                 | 4%              | 45%            | 13%            |                 | 50%     |

If a combination of one or more effects fully explains the difference in OPD between SWI and interface, then \( \beta \) amounts to 100%.

This procedure was applied to literature data available for four marine and three freshwater burrowing organisms. The available data are summarized in Table 4. In all cases, the observed OPD near the burrow \( \delta_{int} \) is substantially smaller than the observed OPD near the sediment-water interface \( \delta_{swi} \). To investigate the cause of this, we used the above procedure and first accounted only for the influence of curvature (based on reported values for the burrow radius \( r_{b} \)). This provides a first value \( \delta_{1} \) for the predicted OPD at the interface using Eq. (15) and an associated value for \( \beta_{1} \) from Eq. (16). Subsequently, we accounted for partial burrow oxygenation (based on data for the concentration in the burrow \( c_{0} \)). This provides a second set of values \( \delta_{2} \) and \( \beta_{2} \). Then finally, we assigned \( \delta_{3} = \delta_{int} \) as the observed OPD near the burrow. Consequently, the effect that could not be explained by the former two mechanisms was ascribed to increased microbial O\(_2\) consumption in the sediment surrounding the burrows. Since no local porosity data was available, we assumed that porosity and diffusivity near the burrows were similar as at the SWI.

The results of these calculations are summarized in Table 4. On average, \( \beta_{1} \sim 50\% \), so about half of the observed OPD reduction can be ascribed to the geometrical effect of
burrow curvature, although there seems to considerable variability between species. For the amphipod *Corophium volutator* (Zorn et al., 2006) curvature alone explains the decrease in OPD. For the other species, the contribution of curvature ranges from 29% in *Sialis velata* to 81% in *Hexagenia limbata*. For the data analyzed here, the effect of reduced burrow oxygenation ($\beta_2$) was small, because most data were collected in the upper part of the burrows, where O$_2$ levels were similar to the overlying water. For *Sialis velata*, the reduced O$_2$ concentration in the burrow water contributed 19% to the observed reduction in the OPD. The remaining effect ($\beta_3$), we ascribed to increased microbial activity and hence increased O$_2$ consumption near the burrow wall. On average, this contributed 45% to the observed OPD reduction (range 0–67%). From this, we could calculate the required increases in the O$_2$ consumption (expressed as 100$\times$ $R_{int}$/$R_{swi}$). On average, $R_{int}$ was estimated to be 13% larger than $R_{swi}$ (range 0–26%). Overall, this appears a relatively modest increase of the reactivity near the burrow wall.

c. Factors controlling the oxygenated volume in irrigated sediments

An analogous sequential modelling procedure can be used to examine the controls on the irrigated volume

$$V_{irr}^{model} = \left( \frac{V_{irr}^{G+C}}{V_{irr}^{C}} \right) \left( \frac{V_{irr}^{C}}{V_{irr}^{A}} \right) \left( \frac{A_{int}}{A_{swi}} \right) V_{ox}^{swi} \tag{17}$$

The quantity $V_{ox}^{swi} = A_{swi} \delta_{swi}$ represents the oxygenated volume at the sediment water interface, and so the factor $A_{int}$/$A_{swi}$ accounts for surface area extension. The $V_{irr}^{G+C}$/$V_{irr}^{C}$ accounts for the effect of local geochemistry on the irrigated volume, while $V_{irr}^{C}$/$V_{irr}^{A}$ accounts for curvature. This modeling procedure was applied to investigate the controls on the oxygenated volume in sediments inhabited by burrowing macrofauna (Table 5), as well as for two vascular plants with rhizome networks (Table 6).

For the burrowing macrofauna, we considered three representative faunal communities of coastal sediments: a population of adult *Nereis diversicolor*, a population of *N. diversicolor* juveniles, and a population of *Arenicola marina* adults (Kristensen, 2000). Representative organism densities and burrow geometries were adopted (Table 5). Furthermore, it was assumed that the geochemical conditions at the SWI and burrow interface were comparable in all three populations, with an oxygen penetration depth $\delta_{swi}$ of 3 mm. Since our aim was primarily to investigate the effect of burrow curvature, we ignored partial oxygenation of the burrow and/or stronger microbial activity in the burrow wall (there are few data on the actual levels of oxygenation within burrows under natural conditions). Also, when calculating the oxygenated volume due to irrigation, we only consider the effect of radial oxygen diffusion through the burrow walls. In the case of *Arenicola*, the advective injection of burrow water into sediment represents another important mechanism of bio-irrigation (Meysman et al., 2006), which additionally contributes to $V_{ox}^{bio}$, and may account for half
Table 5. Factors controlling the oxygenated volume in three communities of burrowing fauna: *Nereis diversicolor* (adults), *Nereis diversicolor* (juveniles), *Arenicola marina*.

<table>
<thead>
<tr>
<th></th>
<th>Nereis (adult)</th>
<th>Nereis (juv)</th>
<th>Arenicola</th>
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<tbody>
<tr>
<td>Density</td>
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<td>Burrow radius</td>
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<td>Burrow length</td>
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<td>Burrow volume</td>
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<td>Length scale SWI</td>
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<tr>
<td>Length scale INT</td>
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<tr>
<td>OPD at SWI</td>
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<tr>
<td>OPD at burrow</td>
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<tr>
<td>Curvature effect</td>
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<tr>
<td>Oxygenated volume SWI</td>
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<tr>
<td>Irrigated volume</td>
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<td>Volume ratio</td>
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<tr>
<td>Upscaling error</td>
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</table>

Table 6. Factors controlling the oxygenated volume in three plant communities: seagrass (*Zostera marina*) and common reed (*Phragmites australis*). Parameters for *Zostera marina* are taken from (Terrados et al., 1999), (Jensen et al., 2005) and (Frederiksen and Glud, 2006). Parameters for *Phragmites australis* are taken from (Armstrong and Armstrong, 2001) and (Beckett et al., 2001).

<table>
<thead>
<tr>
<th></th>
<th>Zostera marina</th>
<th>Phragmites australis</th>
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</thead>
<tbody>
<tr>
<td>Density</td>
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<tr>
<td>Root tip radius</td>
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<tr>
<td>Area extension</td>
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<tr>
<td>Root tip volume</td>
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<tr>
<td>Length scale SWI</td>
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<td>Length scale INT</td>
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<tr>
<td>OPD at SWI</td>
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<td>OPD at root tip</td>
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<td>Curvature effect</td>
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<tr>
<td>Oxygenated volume SWI</td>
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<tr>
<td>Irrigated volume</td>
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<tr>
<td>Volume ratio</td>
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<td>Upscaling error</td>
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</table>
Nereis respectively (many small burrows). The latter values fall well within the range 1.3–5 that has been reported for nereid populations in the field (Davey, 1994; Kristensen, 2000; Nielsen et al., 2004). The presence of bio-irrigating organisms increases the oxygenated volume substantially. The oxygenated volume associated with bio-irrigation accounts for 31% (Arenicola), 78% (adult Nereis) and 85% (juv. Nereis) of the total oxygenated volume. These values reveal that increased surface area created by the burrow structures is the dominant factor controlling the irrigated volume, but that also curvature plays an important role. In the case of Arenicola, the effect of burrow curvature is very small (18%) because of the large burrow radius. Yet, in the case of juvenile nereid population (many small burrows), curvature enhances the surface area effect by 78%, which is substantial.

A similar exercise was carried out to investigate oxygenation due to oxygen release from root tips. A representative parameter set (Table 6) was collected for the root system of two aquatic plant communities: the seagrass *Zostera marina* (Terrados et al., 1999; Jensen et al., 2005; Frederiksen and Glud, 2006) and the common reed *Phragmites australis* (Armstrong and Armstrong, 2001; Beckett et al., 2001). Although these plants have cylindrical roots, the oxygen release is typically concentrated within a small zone near the root apex, which we approximate as a spherical interface. In contrast to burrow networks, the presence of root systems does not seem to greatly increase the oxygenated volume of the sediments (6% in Zostera and 4% in Phragmites). However, because of the small size of the root tips, there is a large effect of curvature on the oxygenated volume. In the case of Zostera (with a small 0.1 mm root radius), curvature increases the oxygenated volume by nearly a factor of nine, while in the case of Phragmites, this becomes a factor of three. Accordingly, the effect of curvature is much more pronounced in the oxygen loss from root systems when compared to burrow networks. Note that the localized oxygen release at root tips, as shown by Zostera and Phragmites, is not typical for all submersed macrophytes. Many brackish/freshwater species, like Potamogetons and isoteids, show oxygen release over a much larger zone of their roots, resulting in much higher oxygen release rates and hence, larger oxygenated volumes than the 4–6% reported above (Sand-Jensen et al., 1982; Laskov et al., 2006). As noted above, the Zostera and Phragmites were selected to illustrate the use the spherical model equations in the context of $O_2$ release from roots.

d. Sensitivity analysis

In the previous sections we found that curvature can have a large impact on the oxygen penetration distance and the oxygenated volume in aquatic sediments. However, curvature is not always important (e.g. the Arenicola burrows above), and so, it would be valuable to have a rule of thumb, as to know whether the simple area upscaling procedure as detailed above can be used used or not. To this end, we performed a sensitivity analysis of this curvature effect. The expressions in Table 2 show that the OPD near a curved interface is governed by two fundamental length scales. One length scale defines the interface geometry (the source radius $r_s$), while the other length scale combines all essential parameters influencing the
Figure 4. Influence of the radius on the oxygen penetration near the cylindrical burrow. (a) Radial concentration profiles for selected values of the burrow radius; (b) The oxygen penetration distance $\delta = r_s - r_0$ as a function of the burrow radius $r_s$. All concentrations and distances are plotted in non-dimensional form: $c(r)/c_0$, $\delta/\lambda_{int}$ and $r_s/\lambda_{int}$. The triangle and circle denote the Arenicola and juvenile Nereis as in Table 5 (see text).

local geochemistry of oxygen (the geochemical length scale $\lambda$ or $\xi$). Here we concentrate solely on the influence of the source radius, assuming that the geochemical climate round the interface is similar to that at the SWI. Under these conditions, one can easily show that (1) the interface OPD is always smaller than that of the planar case (i.e., $\delta_{int} < \delta_{swi}$), and that (2) when the source radius becomes large, the OPD approaches that of the planar case (i.e., $\delta_{int} \rightarrow \delta_{swi}$ when $r_s \rightarrow +\infty$).

Figure 4a shows a sequence of radial concentration profiles for the cylindrical case. The values of (dimensionless) burrow radius $r_s/\lambda_{swi}$ range from 0.01 to infinity. The lower limit 0.01 corresponds to a burrow radius of 0.5 mm and an oxygen penetration depth of 50 mm at the SWI. Exploring lower values for $r_s/\lambda_{swi}$ is not realistic, as either the burrow radius becomes too small, or the sediment becomes completely oxygenated. The sequence of profiles displays a clear trend. When the burrow radius increases, the radial $O_2$ profile drops less sharply. Ultimately, when the burrow radius becomes much larger than the planar OPD (i.e., when $r_s > \delta_{swi}$), the “cylindrical” profile approaches the “planar” profile, as required by theory.

Figure 4b plots the relationship between the OPD ratio $\delta_{int}/\delta_{swi}$ versus the (dimensionless) burrow radius $r_s/\lambda_{swi}$. This OPD ratio becomes closer to one when the burrow radius increases. Values for typical bio-irrigating fauna (Arenicola and Nereis) are indicated. The OPD attains 90% of the planar limit when the burrow radius is about as large as the planar OPD, i.e., $r_s \approx \lambda_{swi}$. This can be used as a criterion for model complexity. When a 10% error is acceptable, the length scale $\lambda_{swi}$ can be regarded as a threshold to decide whether a simplification from the cylindrical to the planar model is justified or not. When the burrow radius is larger than $\lambda_{swi}$, the deviation between the cylindrical and the planar geometries...
becomes small. In this case, the burrow surface can be treated as a flat interface without introducing a major bias. However, when the burrow radius is smaller than $\lambda_{swi}$, a significant bias is introduced when using the planar expressions, and hence, one should stick to the more complex cylindrical expressions in Table 2 and 3. If one imposes a more stringent error tolerance, the threshold length scale has to be adapted accordingly. For example, to reach 99% of the planar OPD, the dimensionless burrow radius must increase to the value $r_s \approx 16 \times \lambda_{swi}$ (i.e., the actual burrow radius should 16 times larger than the OPD at the sediment-water interface).

The situation for spherical root tips is entirely analogous to the cylindrical case. When the geochemical climate round the burrow is similar to that at the SWI (1) the OPD is always smaller than in the planar case, and (2) the OPD approaches that of the planar case when the source radius increases. The radial $O_2$ distributions depicted in Figure 5a confirm this. Moreover, Fig. 5b shows how the (dimensionless) oxygen penetration distance varies with the (dimensionless) sphere radius $r_s$. The OPD reaches 90% of the planar limit when the dimensionless sphere radius $r_s \approx 2.6 \times \lambda_{swi}$. Note that this is significantly larger than in the cylindrical case (where $r_s \approx \lambda_{swi}$). For the OPD to reach 99% of the planar one, the dimensionless sphere radius must be $r_s \approx 33 \times \lambda_{swi}$ (compare to the corresponding value 16 for the cylindrical case).

Figure 6 shows how curvature affects the irrigated volume (the factor $\gamma_{int}$ is plotted as a function of the radius $r_s/\lambda_{swi}$). These results again show that curvature becomes important when the radius $r_s$ becomes progressively smaller. For sufficiently large radii, $\gamma_{int}$ approaches one. Only in this case, the interfaces form a “simple” extension of the SWI (provided that geochemical climate between burrows and SWI is also similar). These
Figure 6. Influence of curvature on the oxygenated volume and irrigational oxygen uptake rate in sediments. (a) Cylindrical geometry (burrows): The curvature factor $\gamma_b$ as defined in Table 3 is plotted as a function of the dimensionless radius $r_b/\lambda_{int}$. (b) Spherical geometry (root nodules): The factor $\gamma_r$ as defined in Table 4 is plotted as a function of the dimensionless radius $r_r/\lambda_{int}$. The triangle and circle denote two example populations of bio-irrigating organisms (panel a) or rooting vascular plants (panel b).

results are very similar to those obtained when analyzing the effect of curvature on the OPD (Figs. 4 and 5). One cannot define an “absolute” critical radius above which curvature can be ignored. Instead, a relative criterion decides when curvature becomes important. Using a 90% tolerance level, curvature becomes important when the dimensionless radius $r_s/\delta_{swi}$ becomes smaller than 2.9 and 5.9 in the cylindrical and spherical case respectively.

5. Discussion

a. Influence of curvature on oxygenated volume and IOU

Given the importance of oxygen dynamics in sediment biogeochemistry, there has been considerable interest in an accurate calculation of oxygen fluxes and consumption rates. One aspect that has been thoroughly investigated is the influence of (micro-)topography on the diffusive oxygen uptake (DOU) at the sediment-water interface (Jorgensen and Marais, 1990). If one applies the one-dimensional form of Fick’s law to a micro-electrode profile at the sediment surface in order to obtain a DOU value, one implicitly treats the SWI as an infinitely flat plane. However, the sediment surface shows curvature and undulations across a range of scales, and hence, several studies have targeted the discrepancy between the exchange at a flat plane versus a sediment with topography (Jorgensen and Marais, 1990; Roy et al., 2002, 2005). A detailed sub-millimeter characterization of the sediment surface has shown that true fluxes at the SWI may differ by 10-20 % from diffusive model calculations that treat the SWI as a perfectly flat interface (Roy et al., 2002, 2005).

Here we have studied a similar “curvature” effect on diffusive fluxes, though now at internal interfaces within aquatic sediments, that is burrow walls and root tips. The oxygen
uptake at these internal interfaces is referred to as the irrigational oxygen uptake (IOU). In nearshore sediments, the IOU provides an important contribution in the TOU (Glud et al., 2003). To accurately calculate the IOU, one requires the oxygen penetration distance $\delta_{int}$ at the burrow or root interface (see expressions in Table 4). Yet, data on $\delta_{int}$ are typically scarce, as the oxygen consumption and penetration around biological structures is hard to measure (as discussed above). Therefore, it is tempting to ignore the effect of curvature, and to regard the internal interfaces as a simple linear extensions of the sediment-water interface. By ignoring the curvature factor in (setting $\gamma_s = 1$ in Eqs. (8) and (12)), one arrives at

$$\delta_{int} \approx \delta_{swi}$$ \hspace{1cm} (18)

$$\text{IOU} \approx \left( \frac{A_{int}}{A_{swi}} \right) \cdot \text{DOU}$$ \hspace{1cm} (19)

$$V_{irr}^{ox} \approx \left( \frac{A_{int}}{A_{swi}} \right) \cdot V_{swi}^{ox}.$$ \hspace{1cm} (20)

Because DOU and $\delta_{swi}$ are relatively easy to measure, these expressions can be readily applied in back of the envelope calculations. Therefore, a crucial question is if and when these “planar” approximations are justified?

Our model analysis revealed the conditions under which curvature strongly influences the estimation of key properties around biological structures (oxygen penetration distance, oxygenated volume, irrigational oxygen uptake). When neglecting the effect of curvature, one may substantially underestimate the irrigational oxygen uptake and oxygenated volume within the sediment (Figs. 4, 5 and 6). Example calculations show that for typical infauna populations, the error may range up to 60% (Table 5 - Fig. 6), while in the case of seagrass root tips, this may even approach a 1000% (Table 6 - Fig. 6). Accordingly, the effect of curvature at internal interfaces is much more pronounced than that induced by microtopography at the sediment-water interface.

The effect of curvature is non-linearly dependent on the radius $r_s$ of the burrow or root tip. The effect becomes stronger when the radius $r_s$ decreases (Figures 4, 5 and 6). As a general “rule of a thumb”, the radius $r_s$ of the biological structure must be larger than $\delta_{swi}$ to safely neglect geometrical corrections. The actual critical ratio $r_s / \delta_{swi}$ depends on the tolerance level, the geometry (cylindrical or spherical), and whether one examines the OPD or the oxygenated volume/IOU (a summary is provided in Table 7). Below these values, the planar approximations (Eqs. 18–20) can substantially overestimate the OPD, and underestimate the oxygenated volume and IOU near burrows and roots.

b. Factors controlling the OPD near burrow walls

When all parameters other than geometry are the same, our model analysis predicts that the curved OPD is always lower than the corresponding planar value, and that when the curvature becomes weak, the OPD approaches the planar value (Figs. 4, 5). This is fully
Table 7. Summary of the effect of curvature on biogeochemical properties. Critical values for the ratio \( \frac{r_s}{\delta_{swi}} \) are given, where \( r_s \) is the radius of the biological structure (burrow or root), and \( \delta_{swi} \) is the oxygen penetration depth at the sediment-water interface. Above these critical values the bias due to curvature is less than 10%, and hence, the effect of curvature can be ignored in the calculation of the biogeochemical property.

<table>
<thead>
<tr>
<th>Biogeochemical property</th>
<th>Cylindrical</th>
<th>Spherical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxygen penetration distance</td>
<td>OPD</td>
<td>1.1</td>
</tr>
<tr>
<td>Oxygenated volume</td>
<td>( V_{ox}^{int} )</td>
<td>2.8</td>
</tr>
<tr>
<td>Irrigational oxygen uptake</td>
<td>IOU</td>
<td>2.8</td>
</tr>
</tbody>
</table>

consistent with previous simulations of radial oxygen profiles near burrows (Aller, 1988; Fenchel, 1996), albeit with different model assumptions. The prime cause is a surface-to-volume effect: at strong curvature, the volume of surrounding \( O_2 \)-consuming sediment per unit interface area becomes larger.

In recent years, this reduction of the \( O_2 \) penetration near curved interfaces has been experimentally confirmed in micro-electrode studies of near ventilated burrows of freshwater and marine infauna (data compiled in Table 5). These studies indeed show that OPD values around the burrows are systematically smaller as compared to the sediment-water interface. In the past, a number of causes have been proposed to explain this observation: (1) curvature of the burrow interface as previously discussed (Aller, 1988; Fenchel, 1996), (2) a lower oxygen concentration in the burrow water compared to the overlying water (Fenchel, 1996) (3) reduced porosity and/or diffusivity in the burrow lining (Aller, 1983; Hannides et al., 2005), or (4) increased microbial activity, leading to higher consumption rates \( R_{int} \) near the burrow wall (e.g., Stief et al. 2004; Zorn et al. 2006). The analysis presented here allows to distinguish these various effects (see Eqs. 13 to 17). Roughly half of the observed decrease in the OPD can be attributed to curvature, the other half is mainly due to increased \( O_2 \) consumption in the sediment surrounding the burrows (Table 4). Our calculations indicate that the \( O_2 \) consumption near the burrow is on average 13% higher than at the sediment-water interface.

Note however that the current dataset on radial \( O_2 \) profiles near burrows is very limited, and so our results must be considered as tentative. Particularly, the reported \( O_2 \) levels in the burrow water are all close to the value in the overlying water, which seems not really representative for actual burrow systems. Other studies, measuring the \( O_2 \) at the outlet of burrow, have shown a greater oxygen depletion in the outflowing burrow water (Munksby et al., 2002; Wenzhofer and Glud, 2004). This discrepancy could be due to a bias in the method employed. Micro-electrode studies typically target the upper (easy reachable) part of the burrow where burrow water still has higher \( O_2 \) levels. A second bias of micro-electrode studies might be related to burrow size. The present dataset is geared towards larger burrow systems that are more easily amenable to experimentation. One would expects that because of the surface-to-volume effect, small (< 1 mm) burrow systems (1) show more depleted \( O_2 \) levels in the burrow water (more difficult to remain oxygenated) and (2) that the curvature
effect is much more important, decreasing the O$_2$ penetration around these small burrows (Fenchel, 1996).

c. Factors controlling the oxygenated volume

Our analysis (Eq. 8) shows that benthic fauna influence the irrigated volume in three principal ways: (1) Surface area: burrow walls increase the area exposed to oxygen relative to the sediment-water interface (2) Burrow climate: geochemical properties like porosity, diffusivity, reactivity, and interface concentration may differ near the burrow wall as compared to the SWI (3) Burrow geometry: burrow interfaces display curvature. Note that the influence of burrow climate counteracts that of curvature. Strong curvature in small burrows increases the oxygenated volume, while enhanced microbial activity in burrow linings, and partial flushing of burrows, both decrease the oxygenation of the burrow lumen, and hence, they reduce the oxygenation of the sediment.

Reported estimates for the fraction of the oxic sediment volume attributed to burrow structures are 2–10% in the Barents Sea (Jorgensen et al., 2005), 6–16% in Danish harbour sediments (Fenchel 1996), and 54–70% in a sediment heavily bio-irrigated by Nereis diversicolor (Wenzhöfer and Glud 2004). One question is how to explain this apparent variability. To end this end we examined three typical coastal communities: Nereis juveniles, Nereis adults and Arenicola. The oxic microzones caused by diffusion from burrows respectively accounts for 77%, 68% and 22% of the total oxygenated sediment. Note that in the case of Arenicola there will be additional oxygenation due to advective pumping of oxygenated burrow water into the sediment surrounding the distal part of the burrow.

These results show that irrigational sediment oxygenation strongly depends on various characteristics of the faunal community, such as community composition, life history stage, abundance and size of the individuals. Therefore, parameters like population biomass or total burrow volume may be poor estimators of the actual irrigational sediment oxygenation. Although the burrow volume generated by the juvenile Nereids is only 1.5 times that created by Arenicola, the oxygenated volume around the burrows is 12 times larger, which is considerable. Instead we advocate a more mechanistic approach that is based on three biological parameters (burrow radius, burrow density, area extension - see Tables 5). Based on the irrigating fauna present, this can cause of significant variation between apparently similar sites in biogeochemical process rates that are directly dependent on oxygen, such as organic matter processing.

In conclusion, this study provides a systematic presentation of the mathematical equations governing the oxygen distribution near sedimentary microniches such as burrows and macrophyte roots. Currently, experimental data on the O$_2$ distribution around these microniches is still limited. However, new developments, such as planar optode sensors, should enable an improved access to such data providing increased spatial coverage and detail. The model toolbox presented here could facilitate the interpretation of such data, and stimulate the quantitative investigation of the factors controlling the oxygen penetration distance (OPD) and the oxygenated volume around roots and burrows.
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