

7 Appendix: A note about non-local irrigation models

Boudreau (1984) demonstrated that a one dimensional diffusion model with a non-local source/sink term can be mathematically equivalent to radially integrating Aller's cylinder model, which provided a very useful method for including bioirrigation into one-dimensional diagenesis models. Limitations to the technique have been known for some time. For example:

This type of model is extremely useful in describing, for example, average NH_4^+ distributions in bioturbated deposits, but does not readily describe the effects of boundary reactions such as burrow wall nitrification, and interactions such as denitrification/nitrification balances resulting from specific geometries. (Aller (1988) p. 329)

Aller (2001) discussed these limitations also, concluding that a non-local model is only a good replacement for a full cylinder model (or a more general microenvironment model) if there is no radial dependence of reaction or transport properties (ie. reaction zonation around burrows cannot be important) and if the reaction kinetics are linear. Clearly these requirements are violated in multi-component diagenetic models, which consist of multiple species interacting in non-linear ways.

In gauging whether to use a non-local model for the irrigation modelling in Chapter 5, I explored the difference between the cylinder and non-local models for some specific examples.

7.1 Background

Aller's cylinder model equation is:

$$\frac{\partial C}{\partial t} = D_s \frac{\partial^2 C}{\partial z^2} + \frac{D_s}{r} \frac{\partial}{\partial r} r \frac{\partial C}{\partial r} + R(C, z, r) \quad (7.1)$$

where z is vertical distance from the sediment surface, r is the horizontal distance from the burrow centre, C is the concentration, D_s is the molecular diffusion coefficient corrected for tortuosity and R is a reaction term.

Typical boundary conditions are

$$\begin{aligned}
 C &= C_0 & z &= 0 \\
 C &= C_0 & r &= r_1 \\
 \frac{\partial C}{\partial r} &= 0 & r &= r_2 \\
 \frac{\partial C}{\partial z} &= B & z &= L
 \end{aligned} \tag{7.2}$$

where r_1 is the radius of the burrow, r_2 is the outer radius of the solid annulus surrounding the burrow and L is the depth of the burrow. B represents a prescribed flux at the base of the burrowed zone.

Following Boudreau (1984), equation (5.1) can be multiplied by $r/(r_2^2 - r_1^2)$ and integrated laterally to give,

$$\frac{\partial \bar{C}}{\partial t} = D_s \frac{\partial^2 \bar{C}}{\partial z^2} - \frac{2D_s}{r_2^2 - r_1^2} r_1 \left. \frac{\partial C}{\partial r} \right|_{r=r_1} + \overline{R(C, z, r)} \tag{7.3}$$

where the laterally averaged concentration is defined as

$$\bar{C} = \frac{2\pi \int_{r_1}^{r_2} r C dr}{2\pi \int_{r_1}^{r_2} r dr} = \frac{2 \int_{r_1}^{r_2} r C dr}{(r_2^2 - r_1^2)} \tag{7.4}$$

and the laterally averaged reaction term is

$$\overline{R(C, z, r)} = \frac{2 \int_{r_1}^{r_2} r R(C, z, r) dr}{(r_2^2 - r_1^2)} \tag{7.5}$$

Boudreau (1984) made the assumption that $\left. \frac{\partial C}{\partial r} \right|_{r=r_1}$ can be approximated by

$$\left. \frac{\partial C}{\partial r} \right|_{r=r_1} \approx \frac{\bar{C} - C_0}{\bar{r} - r_1} \tag{7.6}$$

where $\bar{r}$ is the (unknown) point at which $\bar{C}$ occurs ($r_1 < \bar{r} < r_2$). Figure 7.1 illustrates the approximation.

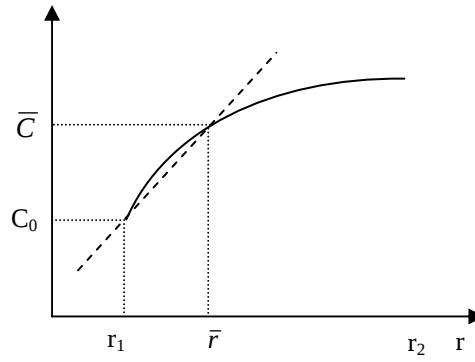


Figure 7.1 The approximation made in equation (7.6). The dotted line represents the approximation to the concentration gradient at r_1 .

With the further assumption that $\overline{R(C, z, r)} = R(\overline{C}, z)$, equation (7.3) can be converted to a one-dimensional diffusion equation with a non-local term:

$$\frac{\partial \overline{C}}{\partial t} = D_s \frac{\partial^2 \overline{C}}{\partial z^2} - \alpha(\overline{C} - C_0) + R(\overline{C}, z) \quad (7.7)$$

where

$$\alpha(z, t) = \frac{2D_s r_1}{(r_2^2 - r_1^2)(\bar{r} - r_1)} \quad (7.8)$$

Boudreau's analysis proved to be very useful, as it demonstrated sound physical reasons for employing equation (7.7) as a representation of bioirrigation in one dimensional sediment diagenesis models.

The questions addressed in this chapter are:

- 1) To what extent is the approximation in equation (7.6) valid?
- 2) Equation (7.8) suggests that the coefficient, α , is a function of diffusivity and $\bar{r}$, both of which are functions of the chemical species, and can both be functions of depth. Yet it is common practice simply to use a constant value across many species and at all depths in a model. Does this simplification matter?
- 3) Integrating the reaction term is only possible if reaction kinetics are linear and independent of the concentration of other species. How well does this approach work for a set of coupled non-linear differential equations, as is typical for multiple species diagenesis models?

Each of these questions is answered in the following three sections by making direct comparisons between solutions to the full cylinder model and non-local model. The next two sections draw on cylinder model results from Aller (1980).

Aller (1980) employed the cylinder model with the following reaction term

$$R = k(C_{eq} - C) + R_0 \exp(-\eta z) + R_1 \quad (7.9)$$

to model the sediment-water exchange of SO_4^{2-} , NH_4^+ and Si, where k , R_0 , η and R_1 are empirical constants and C_{eq} is an equilibrium concentration.

The analytical steady state solution to the cylinder model is (Aller (1980)):

$$C(z, r) = C_0 + Bz + \frac{2}{LD_s} \sum_{n=0}^{\infty} \frac{G_n}{\mu_n^2} \left[\frac{U_0(\mu_n r)}{U_0(\mu_n r_1)} - 1 \right] \sin(\lambda_n z) - \frac{2B}{L} \sum_{n=0}^{\infty} \frac{(-1)^n U_0(\mu_n r)}{\lambda_n^2 U_0(\mu_n r_1)} \sin(\lambda_n z) \quad (7.10)$$

where

$$n = 0, 1, 2, \dots$$

$$\lambda_n = \left(n + \frac{1}{2} \right) \frac{\pi}{L}$$

$$\mu_n = \left(k/D_s + \lambda_n^2 \right)^{1/2}$$

$$G_n = \frac{k(C_0 - C_{eq})}{\lambda_n} - \frac{R_1}{\lambda_n} + \frac{(-1)^n k B}{\lambda_n^2} + R_0 \frac{(\eta e^{-\eta L} (-1)^n - \lambda_n)}{(\eta^2 + \lambda_n^2)}$$

$$U_0(\mu_n r) = K_1(\mu_n r_2) I_0(\mu_n r) + I_1(\mu_n r_2) K_0(\mu_n r)$$

and $I_\nu(z)$ and $K_\nu(z)$ are the modified Bessel functions of the first and second kind respectively of order ν .

Aller (1980) set parameters to the values shown in Table 7.1 (with only r_2 used as a fitting parameter) and found excellent agreement between modelled and field profiles. This configuration of the model is used in the next two sections.

Table 7.1 The cylinder model parameters used in Aller (1980).

Variable	SO_4^{2-}	NH_4^+	Si
C_0	14.7 mM	0.0002 mM	0.074 mM
B	-0.1 mM/cm	0.011 mM/cm	0.060 mM/cm
D_s	0.717 cm ² /day	1.33 cm ² /day	0.687 cm ² /day
η	0.36 /cm	0.61 /cm	0
R_0	-0.383 mM/day	0.267 mM/day	0
R_1	-0.061 mM/day	0.0081 mM/day	0
k	0	0	0.2 /day
C_{eq}	-	-	0.577 mM
r_1	0.05 cm	0.05 cm	0.05 cm
r_2	2.1 cm	2.1 cm	2.1 cm
L	15 cm	15 cm	15 cm

7.2 To what extent is equation (7.6) valid?

The solutions to the specific examples used in Aller (1980) are shown in Figure 7.2. The dotted lines in the figures plot $\bar{r}$ (the location of $\bar{C}$ at each depth). For all three chemical species, $\bar{r}$ is located roughly midway between r_1 and r_2 . The radial concentration gradients are steepest at $r = r_1$, and a visual inspection of the data suggests that the concentration gradient between r_1 and $\bar{r}$ is not linear. These observations call into question the validity of the assumption made in equation (7.6).

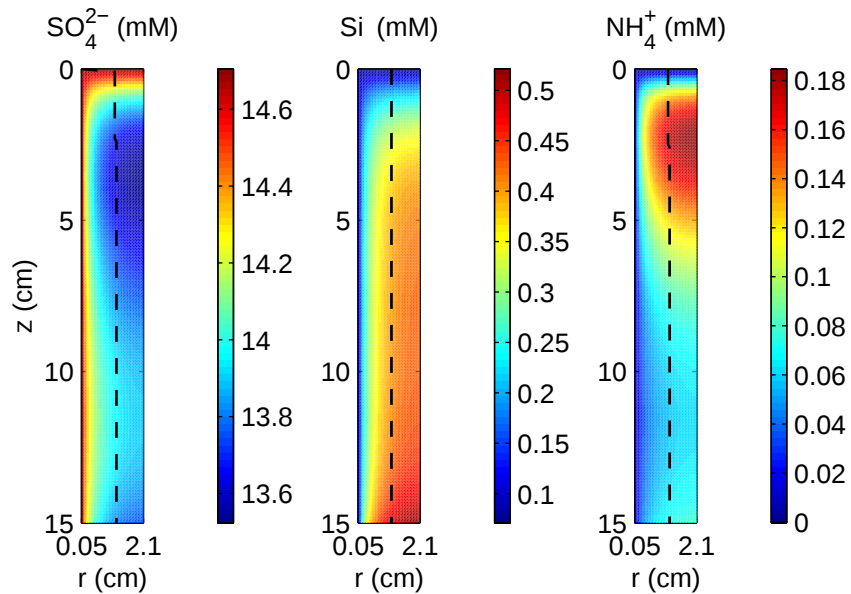


Figure 7.2 Concentration distributions of SO_4^{2-} , Si and NH_4^+ calculated from equation (7.10) using the model parameters in Table 7.1. The dotted line plots $\bar{r}$.

A comparison between the analytical radial derivative at $r = r_1$ and the approximation given in equation (7.6) confirms that in this particular case the approximation is a poor one (Figure 7.3).

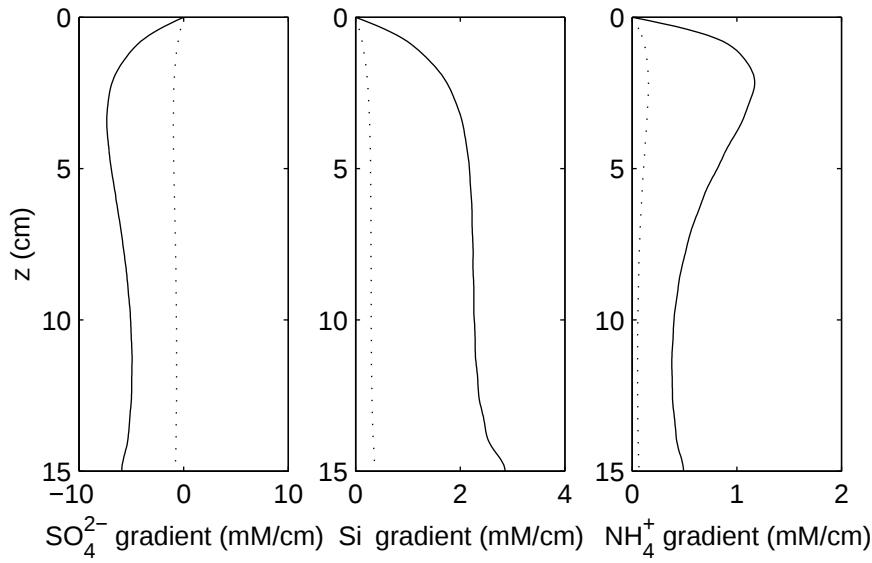


Figure 7.3 Comparison between the analytical radial derivative at r_1 (solid line) and the approximation given in equation (7.6) (dotted line).

Does this poor match matter? Equation (7.8) was used to calculate $\alpha(z)$, and Matlab's 'ode15s' function was used to find a steady state numerical solution to equation (7.7). The solution was compared to the average concentration profiles calculated from the full cylinder model (Figure 7.4).

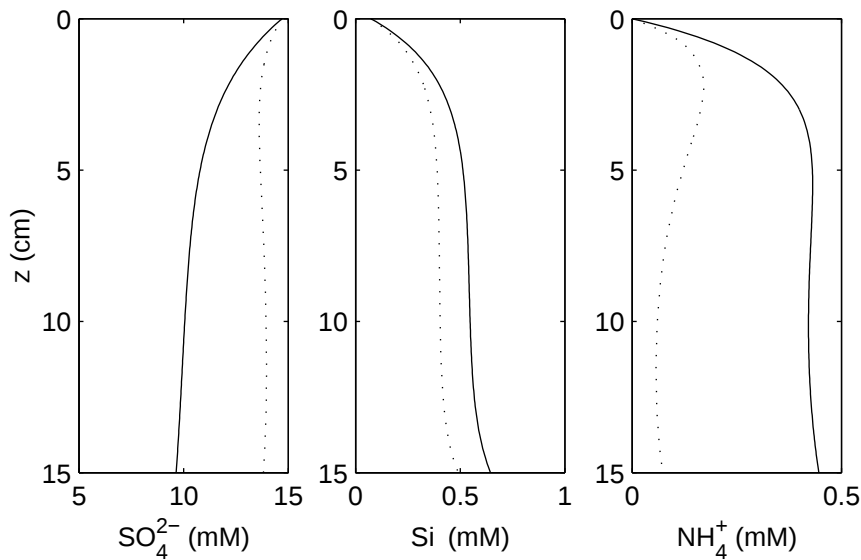


Figure 7.4 Comparison between the average concentration profile calculated from equation (7.10) (dotted line) and the steady state numerical solution to equation (7.7) (solid line). The value of α has been calculated from equation (7.6).

This particular example demonstrates that the approximation given in equation (7.6) is not necessarily a good one. Further, the one dimensional non-local model derived from this approximation can produce significantly different solutions to the radially-averaged concentration profiles generated from the full cylinder model.

7.3 *Validity of using a constant value for α*

The most common implementation of equation (7.7) assumes that α is a constant across all chemical species and at all depths. Values of α are found by calibration against measured profiles, and the expression given in equation (7.8) is rarely used in practice (although it has been used by Furukawa et al. (2000) and Koretsky et al. (2002)). Using this approach for the above example, I found that there are values of α that can be used to generate a very good match to the radially-averaged concentration profile for each species. Values of $\alpha_{\text{SO}_4} = 0.11$, $\alpha_{\text{Si}} = 0.10$ and $\alpha_{\text{NH}_4} = 0.20$ produce profiles which are visually indistinguishable from the radially-averaged analytical solutions. It should be noted that the value of α differs for each species, as predicted by Boudreau's analysis. If the same value of α ($\alpha = 0.14$) is used for all three species, the match between the two models is still good, but less convincing (Figure 7.5). The implication is that the use of a single value of α is not necessarily valid for multiple species models.

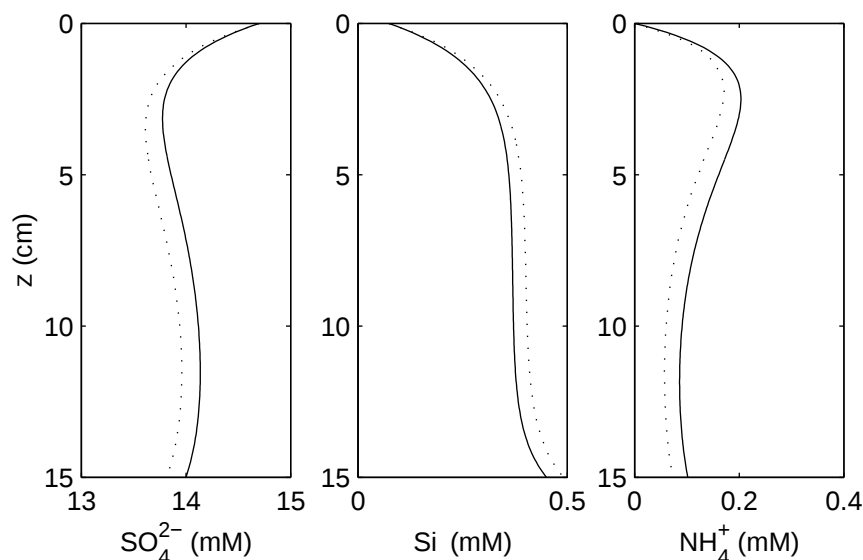


Figure 7.5 Comparison between the average concentration profile calculated from equation (7.10) (dotted line) and the steady state numerical solution to equation (7.7) (solid line). A process of trial and error was used to find a single value of α that provided a good match across all three species ($\alpha = 0.14$).

Given that a useful value of α does exist, I sought to modify Boudreau's formulation slightly by substituting $\bar{r}$ for a value r' such that the approximation in equation (7.6) is true:

$$r'(z,t) = r_1 + \frac{\bar{C} - C_0}{\left. \frac{\partial C}{\partial r} \right|_{r=r_1}} \quad (7.11)$$

The definition of α then becomes:

$$\alpha(z,t) = \frac{2D_s r_1}{(r_2^2 - r_1^2)(r' - r_1)} \quad (7.12)$$

Equations (7.11) and (7.12) were used to calculate r' and α for NH_4^+ , SO_4^{2-} and Si (Figure 7.6). The resulting α profiles match the constant values found earlier (with the exception of the very top and base of the profiles).

The values of r' are roughly the same for each species (to one significant figure accuracy), and so the values of α simply scale with D_s . Other authors have suggested assuming that α values scale with D_s , so that values inferred from one species can be used to calculate the relevant values for other species (eg. Aller and Yingst (1985)). Unfortunately, there is no guarantee that r' will be the same for all species, and so this approach needs to be employed with caution (as noted by Boudreau (1997), p. 143).

These results suggest that cylinder and non-local models could be equivalent if equation (7.11) is used instead of equation (7.6) in the derivation of α . Note that just as equation (7.8) is rarely used by practitioners, equation (7.12) is equally impractical. The replacement of $\bar{r}$ with r' merely represents a minor modification to Boudreau's original derivation, and direct field measurement of r' would not be feasible. It is possible, however, that equation (7.12) could be used in a modelling context. For example, a one-dimensional radial model could be used to estimate $\left. \frac{\partial C}{\partial r} \right|_{r=r_1}$ and $\bar{C}$ at depth. These values could be substituted in to equations (7.11) and (7.12) to derive a value for α which could, in turn, be used to calculate vertical profiles and fluxes. I had hoped to use this approach in my work. Complications involved in multi-species modelling (discussed in the next section) ruled out this possibility in my work; however the approach would be appropriate in many other contexts.

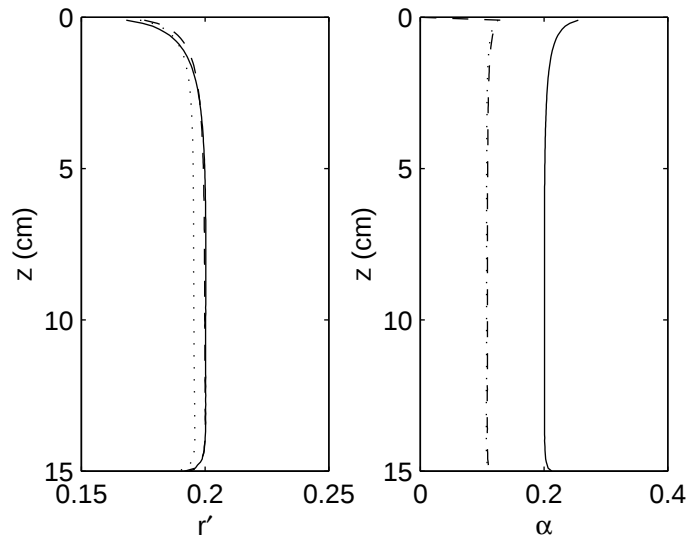


Figure 7.6 Values of r' and a calculated from equations (7.11) and (7.12) (NH_4^+ solid line, SO_4^{2-} dashed line, Si dotted line).

7.4 *Can a non-local model describe a multiple-species system well?*

The analysis so far has been limited to single-species models with reaction terms that are easily integrated radially. Sediment diagenesis models are typically coupled multiple-species models. In such models the reaction terms are more complicated, and because they are dependent on other species' concentrations, they are likely to vary with r . I've used the multiple-species cylinder model from Chapter 5 (see Section 5.6.2) to demonstrate the potential problems of using a radially-averaged approach for such systems.

The model was compared with the one-dimensional models: (1) a diffusion-only radial model (which models a transect radiating out from the burrow wall); (2) a diffusion-only vertical model (which models a vertical profile in sediment with no irrigated burrows); and (3) a non-local vertical model.

The cylinder model was run with the same burrow geometry as earlier examples. A 20-day run was sufficient to bring the cylinder model solution to steady state. P_{DOC} was uniformly distributed with a value of $200 \text{ nmol/cm}^3/\text{d}$ (which corresponds to a carbon mineralisation rate of $25.5 \text{ mmol/m}^2/\text{d}$ for this burrow geometry, assuming P_{DOC} is zero below the burrowed zone of sediment). Figure 7.7 shows the steady state concentration distributions from this configuration. Comparison with the diffusion-only vertical model confirms that irrigation has a strong influence on the radially-

averaged concentration profiles (Figure 7.8). For example, in the cylinder model NH_4^+ escapes through burrow walls as well as the surface and so there is less flux of NH_4^+ to the sediment surface. Consequently, NH_4^+ does not build up to such high concentrations near the sediment surface, and so oxygen can penetrate further. These kinds of interactions between species are not obvious when looking only at tracers with first order decay.

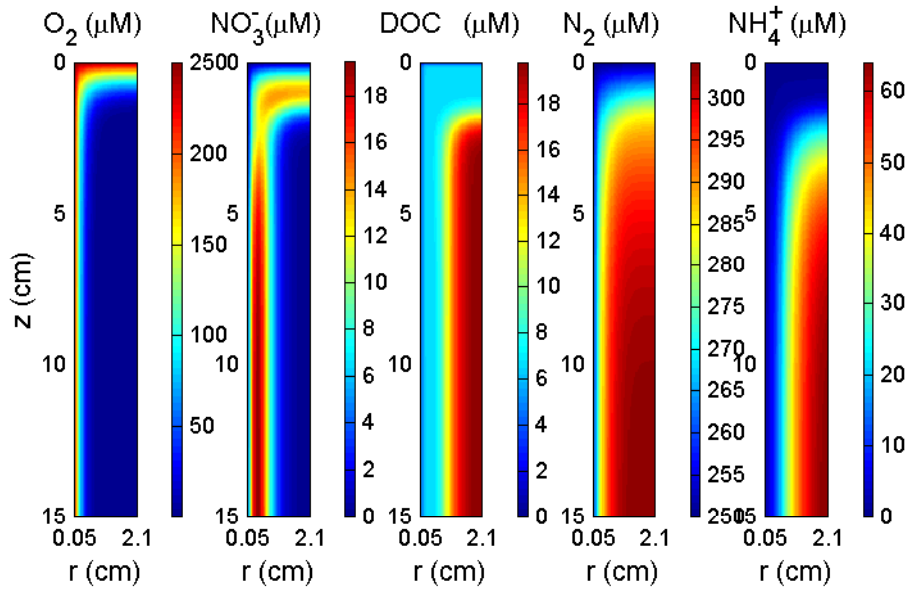


Figure 7.7 Two-dimensional steady state concentration distributions from the 5-species nitrogen cycling model.

The two-dimensional concentration distributions were used to estimate r' using equation (7.11), and these values were used to calculate α from equation (7.12). Unlike in previous examples, both r' and α profiles varied substantially with depth (Figure 7.9 and Figure 7.10). Further, the equations produced negative r' and α values for NO_3^- , DOC and NH_4^+ . Negative values make little physical sense, and so these results suggest that the use of equations (7.11) and (7.12) is inappropriate for this model.

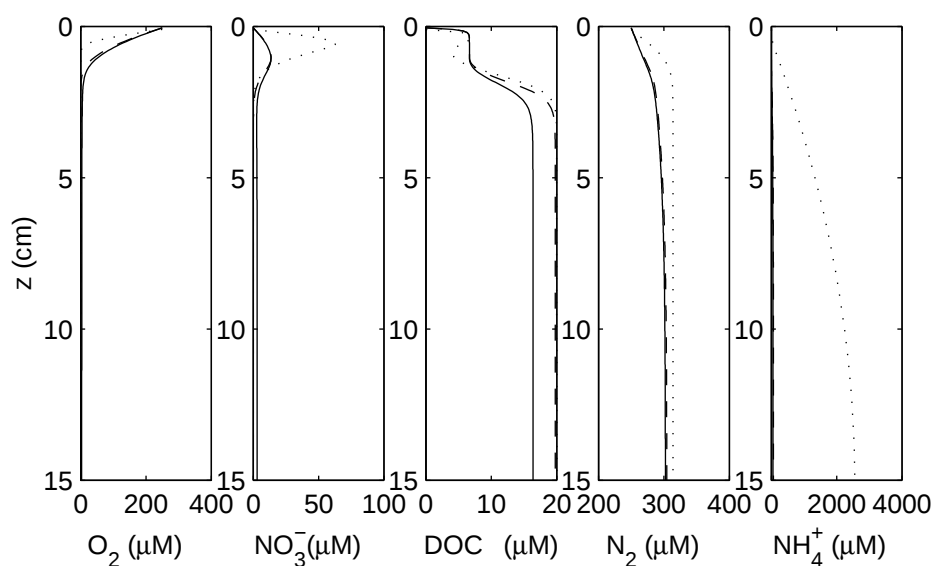


Figure 7.8 Comparison between the two-dimensional model and one-dimensional diffusion-only model. (Solid line: radially averaged profiles from 2D cylinder model; Dotted line: 1D diffusion-only model; Dashed line: vertical profile at $r = r_2$ in 2D cylinder model.) The solid and dashed lines in the NH_4^+ profile are too close to the vertical axis to be clearly visible.

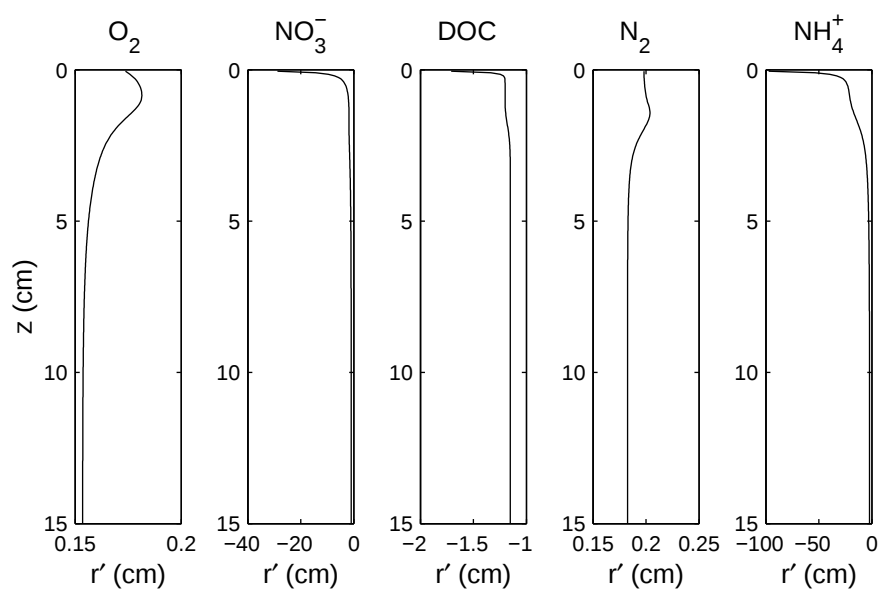


Figure 7.9 Depth variation in calculated values of r' for each species.

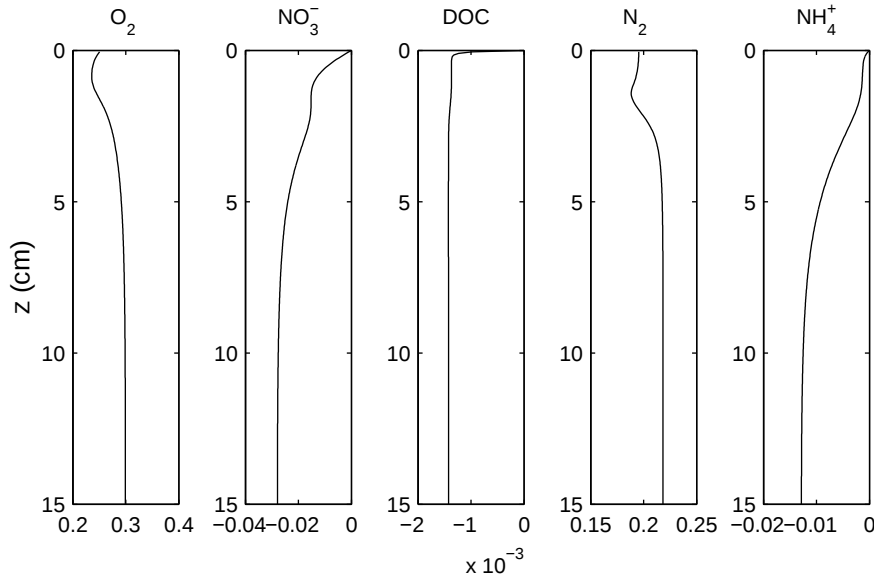


Figure 7.10 Depth variation in calculated values of α (day⁻¹) for each species.

Despite the difficulties in finding a formal derivation of α that ensures equivalence between the cylinder and non-local models, I found that simply substituting the value of r' found in the previous single species examples ($r' = 0.2$) generated a set of α values that produced a good match between the two models (Figure 7.11).

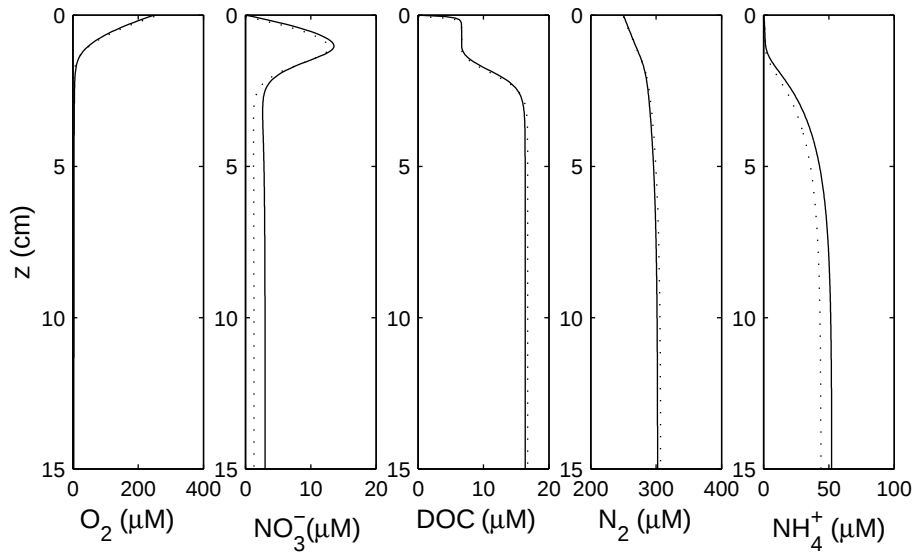


Figure 7.11 Comparison between the cylinder model (solid line) and non-local model (dotted line) profiles.

Equation (7.7) assumes $\overline{R(C,z,r)} = R(\overline{C},z)$, yet in the nitrogen model the reaction terms are coupled and non-linear. A comparison between $\overline{R(C,z,r)}$ and $R(\overline{C},z)$ profiles

demonstrates that they are indeed very different (Figure 7.12), which makes the good match between non-local and cylinder models even more surprising. In fact, although the absolute differences between the non-local and radially-averaged concentrations are low, there are some substantial relative differences between the concentrations for O_2 (and to a lesser extent, NO_3^-). At depth, the radially averaged O_2 concentrations are more than a factor of 7 higher than the non-local values. This difference is enough to ensure that $R(\bar{C}, z, r)$ is much closer to $\overline{R(C, z, r)}$ (Figure 7.12).

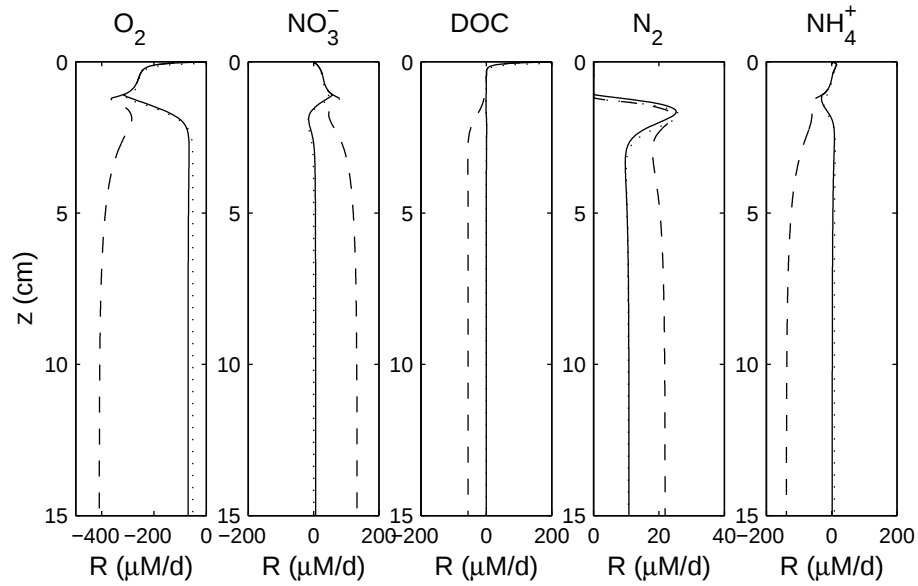


Figure 7.12 Comparison between reaction profiles. Solid line: $\overline{R(C, z, r)}$, where C is the concentration distribution from the cylinder model; Dashed line: $R(\bar{C}, z)$, where $\bar{C}$ is the radially-averaged concentration calculated from the cylinder model; Dotted line: $R(\bar{C}, z)$, where $\bar{C}$ is the concentration profile produced by the non-local model (as shown in Figure 7.11).

The generation of accurate sediment profiles is useful; however, the goal of many sediment diagenesis models is to link the sediment dynamics to the water column by inferring fluxes between the two systems.

The cylinder model flux formulae are (modified from Aller (1980) to represent flux per unit of planar sediment surface):

$$J_{cyl} = J_z + J_r \quad (7.13)$$

where

$$J_z = -\frac{\phi D_s 2\pi \int_{r_1}^{r_2} \frac{\partial C}{\partial z} r \, dr}{2\pi \int_0^{r_2} r \, dr}$$

$$J_r = -\frac{A_r}{A_z} \frac{\phi D_s \int_0^L \frac{\partial C}{\partial r} \, dz}{\int_0^L \, dz}$$

A_z is the surface area of the cylinder top at $x = 0$ and A_r is the surface area of the burrow wall.

If the total flux between the sediment and overlying water is to be predicted from the non-local model, diffusive flux across the sediment boundary and an integrated non-local flux term needs to be included in the calculation:

$$J_{nl} = -\phi D_s \left. \frac{\partial \bar{C}}{\partial z} \right|_{x=0} - \int_0^L \phi \alpha (\bar{C} - C_0) \, dz \quad (7.14)$$

Fluxes predicted from the two-dimensional and non-local models are significantly different for some species (Table 7.2). In particular, the NH_4^+ flux is more than four times higher in the non-local model, and the NO_3^- flux is 30% of the value predicted by the cylinder model.

Table 7.2 Fluxes predicted from the cylinder and non-local models (mmol/m²/day).

	O ₂	NO ₃ ⁻	DOC	N ₂	NH ₄ ⁺
Cylinder model flux (J_{cyl})	-11.4	0.93	0.13	1.34	0.21
Non-local model flux (J_{nl})	-9.51	0.27	0.12	1.34	0.88
J_{nl} / J_{cyl}	0.83	0.29	0.88	1.00	4.11

7.5 Summary

The equivalence between non-local and cylinder models rests on equation (7.8), which in turn relies on the approximation in equation (7.6). Examples drawn from Aller's work demonstrate that even for single-species models this assumption can be invalid. A slight modification corrected this problem (equations (7.11) and (7.12)) and provided

a good match between non-local and cylinder model results. Unfortunately the modified version also broke down when applied to a multiple-species coupled system.

Despite the absence of a formal derivation α of under these circumstances, values of the non-local parameter could still be found to create a good match to radially-averaged cylinder model profiles. The similarity proved to be misleading, however, as the fluxes produced by the two models differed significantly. It would have been inappropriate for me to pursue a non-local irrigation modelling approach in the nitrogen modelling work in Chapter 5, particularly as I was using the model to infer integrated reaction rates and fluxes. It also would have been difficult to justify choices for the non-local parameter, α to reflect other considerations such as partial burrow flushing and time-varying irrigation rates.

It should be emphasised that the non-local irrigation model's performance is lacking only under quite specific circumstances: the application to coupled non-linear reactions. The model remains ideally suited to modelling inert tracers or species with simple reaction kinetics. Further, where higher dimensional modelling is not possible, the non-local irrigation model remains the best approach for one-dimensional modelling. Under these circumstances, it may be useful to implement a one-dimensional radial diffusion model of the kind used in Chapter 5 as well as the vertical non-local model.