Where does Oxygen Extinction Occur in a Soil Profile?

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Abstract: The problem of where and under what circumstances oxygen extinction (concentration in gas phase, $C = 0$) in a soil profile is of increasing interest, due to the effect of nitrous oxide and methane fluxes on atmospheric chemistry (Ravishankara et al., 2009) climate change (Forster et al., 2007). The oxygen concentration profile is also of importance as the biogeochemical processes in soils are mainly mediated by oxidation/reduction reactions.

In soil there are two main sinks for oxygen (O_2), microbes and plant roots. Cook and Knight (2003) developed an analytical model for the steady-state transport of oxygen into a uniform soil by use of transformations of the independent variables, the concentration (C) and spatial dimension (z). The transformed concentration is $C' = C - C_r / \alpha$; C_r is the critical concentration in the water phase at the root surface and α is the Bunsen coefficient. The spatial transform is $X = 2Z_r \exp(-z/2Z_r)\sqrt{g}$ with $g = 2\pi\alpha D_l L_0 / [D_a \ln(R/a)]$, Z_r the scaling depth for an exponentially decreasing root length density with z, D_l is the diffusion of O_2 in soil water, D_a is the diffusion of O_2 in soil air, R is the radius of the root plus saturated soil around the root, a is the root radius and L_0 is the root length density at $z = 0$. This model could not calculate the depth at which either C or C' went to extinction. A subsequent extension was able to calculate the depth (X_1) when $C' = 0$ and the air-filled porosity (θ) was less than a critical value (θ_c) but with the restriction that $dC'/dX\big|_{X_1} = 0$. Here

we remove this restriction and by coupling with model of Cook (1995) where the only O_2 sink is microbes are able to determine the depth (Z_0) at which $C = 0$. This requires solving a set of five boundary condition equations and a recursive method is presented.

The extension to $dC'/dX\big|_{X_1} < 0$ results in essentially the same critical air-filled porosity (θ_c) below which $C' = 0$ at a finite depth. When $\theta < \theta_c$ the recursive method can be used to determine X_1 and from this Z_1. Coupling this with the Cook (1995) solution so that $C = C_r/\alpha$ at Z_1 the remainder of the O_2 profile can be obtained. When θ is less than a further critical value (θ_{z0}) then $C = 0$ at a finite depth and Z_0 can

Figure 1. The depth at which Z_1 or Z_0 occurs as a function of θ for different models for clay soil (Table 1). The critical values of θ are shown.

be determined. An example of a typical result for a silt loam soil is shown in figure 1. This shows the rapid increase in Z_1 and Z_0 that occurs as θ approaches the critical value. The model of Cook and Knight (2013) where $dC'/dX\big|_{X_1} = 0$ (solid circles) overestimates the depth of Z_1 compared to the new model given here which removes this restriction. There is not a perfect match in Z_1 around θ_{z0}, this is likely due to difficulties with computational limitations. This suggests that nitrous oxide generation in particular is likely to occur close to the soil surface in accord with measurements (Clough et al. 2004).

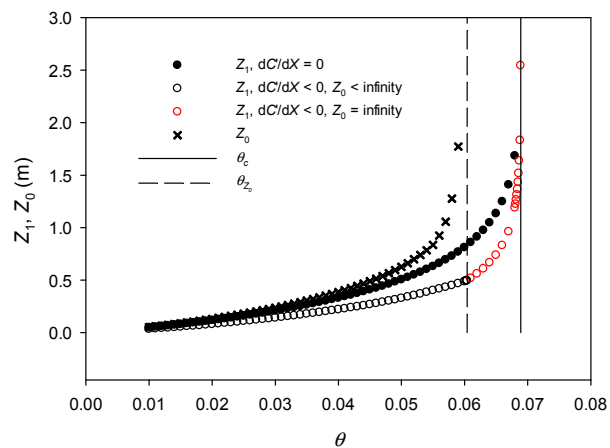*Keywords:* *Oxygen transport, soil aeration, nitrous oxide, methane*

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1. INTRODUCTION

Oxygen is one of the driving forces for biogeochemical processes in soils and understanding the controlling factors in its distribution within soil is important. The main process for oxygen transport into soil is due to diffusion as a result of the sinks for oxygen within the soil. The main sinks are microbial respiration and plant root uptake. Microbial respiration can be described as a distributed sink with decreasing sink strength with increasing soil depth. Uptake by plant roots occurs as a localized transport to the root surface via a zone of saturated soil (Cook and Knight 2003a, b). Via the root length density distribution of the soil this can be converted to a distributed sink, but this sink term now also contains the oxygen concentration (C).

The steady-state oxygen concentration as a function of depth was solved by Cook and Knight (2003a,b) using transforms for both the oxygen concentration $C' = C - C_r / \alpha$ and the spatial dimension $X = 2Z_r \exp(-z / Z_r)\sqrt{g}$. The lower boundary conditions and transformed oxygen concentration meant that the depth at which either $C = 0$ or $C' = 0$ could not be calculated. This was later remedied for $C'(X_1) = 0$ by Cook et al. (2013), but this model could still not find the depth at which $C = 0$ and required $dC' / dX\big|_{X_1} = 0$ as one of the boundary conditions. Here we will present a further extension that removes this boundary condition restriction and by coupling with the model developed by Cook (1995) for only a microbial sink allows the depth at which $C = 0$ (Z_0) to be obtained. We will then show the effect of these changes on critical air-filled porosity values and X_1.

1.1. Theory

Only a limited development of the theory will be given here as the full development has already been published. Using the transforms, the steady-state oxygen transport into soil by diffusion can be described by:

$$\frac{1}{X}\frac{\mathrm{d}}{\mathrm{d}X}\left(X \frac{\mathrm{d}C'}{\mathrm{d}X}\right) = C' + \frac{\beta}{g^p}\left(\frac{X}{2Z_r}\right)^{2(p-1)} \tag{1}$$

where $\beta = M_0 / D_a$, M_0 is the microbial respiration sink strength at $z = 0$, $p = Z_r / Z_m$ is the ratio of exponential scaling depths for the root length density (Z_r) and microbial sink strength (Z_m). For $p = 1$ we obtain the solution:

$$C'(X) = a_1 I_0(X) + b_1 K_0(X) - \frac{\beta}{g}, \quad X_1 \le X \le X_0 \tag{2}$$

where $X_0 = 2Z_r g^{1/2}$, K_0 is a modified Bessel functions of second kind and zero order, I_0 is a modified Bessel functions of first kind and zero order, X_1 is the value of X where $C'(X_1) = 0$ and a_1 and b_1 are parameters that need to be determined. At X_1 the depth (Z_1) can be determined from the definition of X. At Z_1 the concentration of oxygen must be C_r / α from definition of the transformed concentration and further reduction in oxygen concentration can only occur due to microbial respiration. Thus we can now couple the solution from Cook (1995) to give C for $z > Z_1$ (after Cook, 1995):

$$C(z) = C_r / \alpha - \frac{Z_m^2 M_0^*}{D_a}\left[1 - \frac{z^*}{Z_m}\exp\left(\frac{-Z_0^*}{Z_m}\right) - \exp\left(\frac{-z^*}{Z_m}\right)\right], C_r / \alpha < \frac{Z_m^2 M_0^*}{D_a}, 0 \le z^* \le Z_0^*$$

$$= C_r / \alpha - \frac{Z_m^2 M_0^*}{D_a}\left[1 - \exp\left(\frac{-z^*}{Z_m}\right)\right], C_r / \alpha \ge \frac{Z_m^2 M_0^*}{D_a}, 0 \le z^* \le \infty \tag{3}$$

where $z^* = z - Z_1$ and $M_0^* = M_0 \exp(-Z_1 / Z_m)$. From the boundary conditions for eqns (2) and (3) we can get five simultaneous eqns:

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$$A = a_1 I_0 \left(X_0 \right) + b_1 K_0 \left(X_0 \right) - \beta / g$$

$$0 = a_1 I_0 \left(X_1 \right) + b_1 K_0 \left(X_1 \right) - \beta / g$$

$$\left. \frac{dC}{dz} \right|_{Z_1} = \left. \frac{dC'}{dX} \right|_{X_1} \cdot \frac{dX}{dz} = -\left[a_1 I_1 \left(X_1 \right) - b_1 K_1 \left(X_1 \right) \right] g^{1/2} \exp\left(-\frac{Z_1}{2 Z_r} \right)$$

$$\left. \frac{dC}{dz^*} \right|_{Z_1} = -\frac{Z_m M_0^*}{D_a} \left(1 - \exp\left[\frac{-Z_0^*}{Z_m} \right] \right) = \left. \frac{dC}{dz} \right|_{Z_1}, \qquad Z_0^* < \infty$$

$$\left. \frac{dC}{dz^*} \right|_{Z_1} = -\frac{Z_m M_0^*}{D_a} = \left. \frac{dC}{dz} \right|_{Z_1}, \qquad\qquad Z_0^* = \infty$$

$$0 = C_r / \alpha - \frac{Z_m^2 M_0^*}{D_a} \left[1 - \left(\frac{Z_0^*}{Z_m} + 1 \right) \exp\left(-\frac{Z_0^*}{Z_m} \right) \right], \qquad Z_0^* < \infty$$

$$0 = C_r / \alpha - \frac{Z_m^2 M_0^*}{D_a}, \qquad\qquad Z_0^* = \infty \tag{4}$$

where A is the atmospheric concentration of oxygen, K_1 is a modified Bessel functions of second kind and first order, I_1 is a modified Bessel functions of first kind and first order. These set of equations can be solved recursively obtain a_1, b_1, Z_1 and Z_0 using the methodology given below.

2. METHODS

In order to obtain values of Z_1 and Z_0 a scheme to solve the set of constraints in eqn (4). The following schema was devised:

1. Calculate a zero estimate for X_1 using (Cook and Knight, 2013):

   $$X_1^0 \left[I_0(X_0) K_1(X_1^0) + K_0(X_0) I_1(X_1^0) \right] - 1 = \frac{g}{\beta} \left(A - C_r / \alpha \right)$$ and solving iteratively. The

   value of X_1 will lie in the range $X_1^0 < X_1 < X_0$, so the first estimate is $X_1^1 = (X_1^0 + X_0)/2$ and

   $Z_1^1 = -2 Z_r \ln\left(X_1^1 / \left[2 Z_r g^{1/2} \right] \right)$.

2. The values of a_1 and b_1 can now be calculated from the first two constraints in eqn (4) by

   $$a_1 = \left(K_0(X_1^1) \left[(A - C_r / \alpha) + \beta / g \right] - K_0(X_0) \right) / D$$

   $$b_1 = \left(I_0(X_1^1) \left[(A - C_r / \alpha) + \beta / g \right] - I_0(X_0) \right) / D$$

   $$D = I_0(X_0) K_0(X_1^1) - I_0(X_1^1) K_0(X_0)$$

3. The value of $\left. \frac{dC'}{dX} \right|_{X_1^1} \frac{dX}{dz}$ can be calculated with the third constraint in eqn (4) and a first estimate

   of Z_0^{*1} is made by equating the third and fourth constraints of eqn (4)

   $$Z_0^{*1} = -Z_m \left(C_r / \alpha + Z_m \left. \frac{dC'}{dX} \right|_{X_1^1} \frac{dX}{dz} \right) \Big/ \left(\frac{Z_m^2 M_0^*}{D_a} + Z_m \left. \frac{dC'}{dX} \right|_{X_1^1} \frac{dX}{dz} \right).$$

4. The value of $\left. \frac{dC}{dz} \right|_{Z_1^1}$ can be calculated from the fourth constraint in eqn (4).

5. If $\left.\dfrac{dC}{dz}\right|_{Z_1^1} < \left.\dfrac{dC'}{dX}\right|_{X_1^1} \dfrac{dX}{dz}$ or $\left.\dfrac{dC}{dz}\right|_{Z_1^1} > 0$ then $XH = X_1^1$ else $XL = X_1^1$ and

$X_1^2 = (XH + XL)/2$.

This procedure is repeated until $\left|X_1^i - X_1^{i-1}\right| < T$, with $T = 10^{-12}$. If the value of $Z_0 < Z_1$ then constraint 5 is used in calculating $\left.\dfrac{dC}{dz}\right|_{Z_1^1}$ and $Z_0 = \infty$. The values of Z_1 and Z_0 are calculated from X_1 and Z_0^* respectively.

A MatLab computer program was written that solved the above schema for a range of air-filled porosity values. The critical water contents at which $C = 0$ at infinity is estimated with this procedure from the value of D_a by (Cook et al., 2013; Moldrup et al. 2000):

$$D_a = D_a^0 \left(2\theta_1^3 + 0.04\theta_1\right)\left(\frac{\theta}{\theta_1}\right)^{2+3/\lambda} \quad (5)$$

where D_a^0 is the oxygen diffusion in air, θ_1 is θ at a matric potential of -1 m and λ is Campbell (1974) soil water retention parameter. This amends the diffusion in air to that in soil air which is less due to some of the volume being water and solids and the pathway being tortuous. Similarly, the diffusion in the water was calculated with (Olsen et al. 2001):

$$D_l = 1.1D_l^0 \left(f^2 - 0.02\lambda f\right) \quad (6)$$

where D_l^0 is the oxygen diffusion in water and f is the soil porosity. Values of the D_a^0 and D_l^0 can be found in Cook et al. (2013) and the values at 20°C are used in calculations here. The other parameters for the calculations can be found in Cook et al. (2013)

Figure 2. Oxygen concentration (C) with depth for a sandy loam soil at 20°C for different values of θ. The value of $C = C_r/\alpha$ is shown to indicate where $C' = 0$.

3. RESULTS AND DISCUSSION

For sandy loam soil parameters (Table 1) at a temperature of 20° the oxygen concentration profiles with depth for different values of air-filled were calculated with the appropriate model depending on the value of θ for a sandy loam soil at 20°C (figure 2). The extension to values of $C < C_r/\alpha$ using the model developed here is shown for $\theta = 0.11$ where $Z_0 = \infty$ and for $\theta = 0.075$ where $Z_0 = 0.36$ m.

A comparison for Z_1 between the Cook et al. (2013) and eqns (2) and (3) shows that Cook et al. (2013) overestimates the depth at which $C' = 0$ (figure 3). Eqn (3) will give more accurate results as it will represent more closely the actual gradients and sinks in the soil. A comparison of the concentration profiles calculated with Cook et
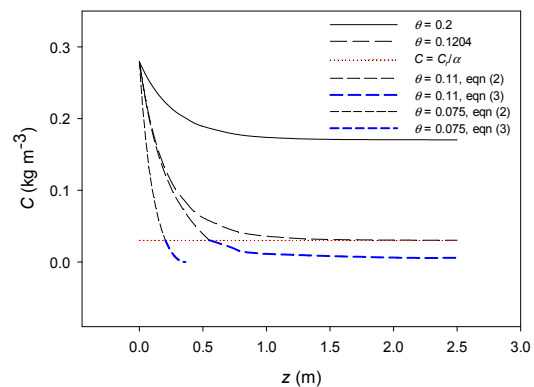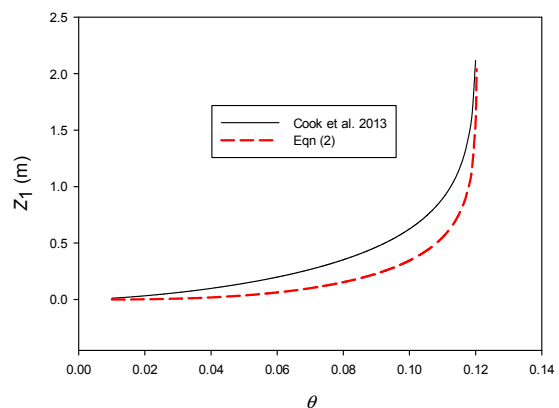

Figure 3. Comparison of Z_1 versus θ for sandy loam soil at 20°C calculated with Cook et al. (2013) and eqns (2) and (3).

al. (2013) and eqns (2) and (3) show how the oxygen profile gets distorted to meet the condition that $dC'/dX|_{X_1} = 0$ with oxygen penetrating to deeper in the soil profile (figure 4). This occurs because in order to meet the boundary conditions oxygen must be consumed so that $C'(X_1) = 0$ and $dC'/dX|_{X_1} = 0$ X_1 must be greater than for eqn (2). This means that for soil biochemical processes such as denitrification and nitrous oxide production the depth at which oxygen concentrations associated with the required redox potential will be close to the soil surface (< 0.2 m) when $\theta < 0.6\theta_c$. This is consistent with measurements of nitrous oxide fluxes to the atmosphere (Clough et al. 2004).

The fact that the depth of oxygen extinction (Z_0) can now be determined with this relatively simple model should also assist in estimating when and where methane fluxes are likely to occur in soil profiles. The increase Z_0 with increase in θ is relatively slow until θ approaches θ_{z0} (figure 1). Again this suggests that the methane generation will be close to the soil surface which will enhance its ability to escape into the atmosphere.

Figure 4. Comparison of oxygen profiles for sandy loam soil at 20°C calculated with Cook et al. (2013) and eqns (2) and (3) with $\theta = 0.1$.

Thus the critical air-filled porosities that can be calculated with eqns (2) and (3) are important in being able to understand soil conditions that could result in nitrous oxide and methane production in soils. The fact that eqns (2) and (3) provide a relatively simple means of calculating soil oxygen concentrations will assist in providing better understanding of many soil biogeochemical processes and help with models that use redox potential as the driver of these processes (Grant, 1999). Critical values for θ for various soils at a temperature of 20°C are presented in Table 1. These results show the general trend of decreasing critical air-

Table 1. Soil properties (after Cook et al., 2013) and critical air-filled porosities (θ_c and θ_{z0}) at 20°C.

Soil	f (m³ m⁻³)	θ_l (m³ m⁻³)	λ	θ_c (m³ m⁻³)	θ_{z0} (m³ m⁻³)
Sand	0.437	0.329	1.69	0.160	0.138
Loamy sand	0.437	0.276	2.11	0.142	0.129
Sandy loam	0.453	0.190	3.11	0.120	0.108
Loam	0.463	0.167	4.55	0.111	0.099
Silt Loam	0.501	0.137	4.74	0.109	0.095
Sandy clay loam	0.398	0.090	4.00	0.089	0.080
Clay loam	0.464	0.090	5.15	0.092	0.081
Silty clay loam	0.471	0.067	6.62	0.082	0.072
Sandy clay	0.430	0.060	5.95	0.076	0.067
Silty clay	0.479	0.054	7.87	0.074	0.065
Clay	0.475	0.047	7.63	0.069	0.060

filled porosities from sand to clay. This may seem at first surprising as sands are generally considered not to have aeration problems. The values need to be considered compared to the θ_l value. This is the value that the soils will drain to. The ratio of θ_c/θ_l for the sand is 0.39 while for the clay is 1.47. This means that the sand will drain to less than θ_c while the clay will require further drying by evapotranspiration before θ_c is reached. Thus these values are consistent with what is common knowledge of soil behavior.

4. CONCLUSIONS

A model for oxygen transport and consumption in soil is present which has two sinks, plant roots and microbial respiration and is able to compute oxygen extinction for transformed and oxygen concentrations. This requires solution of the model of Cook et al. (2013) but without the constraint on the bottom boundary that the gradient in the transformed oxygen concentration (C') is zero when $C'(X_1) = 0$ along with coupling the concentration (C) to the solution of Cook (1995) where microbial respiration is the only sink. A
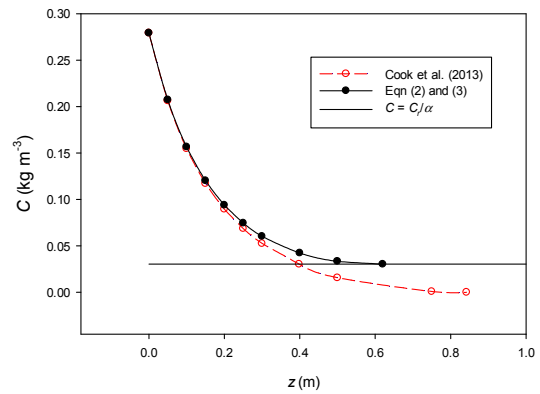
solution scheme is proposed for the five constraints associated with the boundary conditions and it is shown to work. The oxygen concentration for the complete range of oxygen concentrations can now be calculated with this new model.

The depth at which $C'(X_1) = 0$, (Z_1) is less with the new model than that previously calculated with the model of Cook et al. (2013). This means that oxygen concentrations are lower deeper in the soil and this has implications for soil biogeochemical process such as denitrification and methanogenesis. A critical value for the air-filled porosity (θ_c) can be calculated and is essentially the same as that calculated with the Cook et al. (2013) model.

The depth at which $C = 0$ (Z_0) can now be calculated and results show that this, although greater than Z_1, occurs at relatively shallow depths for most the relevant air-filled porosity range. A critical value for the air-filled porosity θ_{z0} can be calculated above which Z_0 is infinite and C is greater than zero for all depths.

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