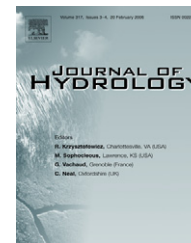




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Critical soil conditions for oxygen stress to plant roots: Substituting the Feddes-function by a process-based model

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Received 20 February 2008; received in revised form 17 July 2008; accepted 20 July 2008

KEYWORDS

Feddes-function;
Gas filled porosity;
Oxygen stress;
Root water uptake;
Transpiration;
Water logging

Summary Effects of insufficient soil aeration on the functioning of plants form an important field of research. A well-known and frequently used utility to express oxygen stress experienced by plants is the Feddes-function. This function reduces root water uptake linearly between two constant pressure heads, representing threshold values for minimum and maximum oxygen deficiency. However, the correctness of this expression has never been evaluated and constant critical values for oxygen stress are likely to be inappropriate. On theoretical grounds it is expected that oxygen stress depends on various abiotic and biotic factors. In this paper, we propose a fundamentally different approach to assess oxygen stress: we built a plant physiological and soil physical process-based model to calculate the minimum gas filled porosity of the soil ($\phi_{\text{gas_min}}$) at which oxygen stress occurs.

First, we calculated the minimum oxygen concentration in the gas phase of the soil needed to sustain the roots through (micro-scale) diffusion with just enough oxygen to respire. Subsequently, $\phi_{\text{gas_min}}$ that corresponds to this minimum oxygen concentration was calculated from diffusion from the atmosphere through the soil (macro-scale).

We analyzed the validity of constant critical values to represent oxygen stress in terms of $\phi_{\text{gas_min}}$, based on model simulations in which we distinguished different soil types and in which we varied temperature, organic matter content, soil depth and plant

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characteristics. Furthermore, in order to compare our model results with the Feddes-function, we linked root oxygen stress to root water uptake (through the sink term variable F , which is the ratio of actual and potential uptake).

The simulations showed that $\phi_{\text{gas_min}}$ is especially sensitive to soil temperature, plant characteristics (root dry weight and maintenance respiration coefficient) and soil depth but hardly to soil organic matter content. Moreover, $\phi_{\text{gas_min}}$ varied considerably between soil types and was larger in sandy soils than in clayey soils. We demonstrated that F of the Feddes-function indeed decreases approximately linearly, but that actual oxygen stress already starts at drier conditions than according to the Feddes-function. How much drier is depended on the factors indicated above. Thus, the Feddes-function might cause large errors in the prediction of transpiration reduction and growth reduction through oxygen stress.

We made our method easily accessible to others by implementing it in SWAP, a user-friendly soil water model that is coupled to plant growth. Since constant values for $\phi_{\text{gas_min}}$ in plant and hydrological modeling appeared to be inappropriate, an integrated approach, including both physiological and physical processes, should be used instead. Therefore, we advocate using our method in all situations where oxygen stress could occur.

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Introduction

Plants need soil oxygen to keep their root metabolism running. Consequently, in water saturated soil conditions, where oxygen diffusion is limited, most terrestrial plants suffer from a lack of oxygen. The effect of insufficient soil aeration on the functioning of plants has been an important field of research for a long time, e.g. in: (1) agriculture, as oxygen stress reduces yields (Dasberg and Bakker, 1970), (2) ecology, since water logging affects plant species composition (Bartholomeus et al., 2008; Burdick and Mendelsohn, 1987; Niinemets and Valladares, 2006; Runhaar et al., 1997), and (3) hydrological modeling, as water logging reduces root water uptake (Feddes et al., 1978).

In reference to the latter field of research, current hydrological models for the unsaturated zone describe soil water flow by solving the Richards' equation, which includes a sink term that represents water uptake by plant roots. Different procedures for the simulation of root water uptake exist (e.g. Doussan et al., 1998; Roose and Fowler, 2004; Van den Berg and Driessen, 2002). A well-known and frequently used procedure to simulate root water uptake, is the reduction function of Feddes et al. (1978). Current hydrological models that include the Feddes-function, such as SWAP (Kroes et al., 2008) and HYDRUS (Šimůnek et al., 2005), compute root water uptake by multiplying potential transpiration (which is determined by meteorological conditions and crop type) with a sink term variable F (Fig. 1). Depending on soil water pressure head h , F corrects for conditions that are either too dry, or too wet. Root water uptake decreases linearly between pressure head h_2 and the anaerobiosis point h_1 due to oxygen stress in wet situations. However, a detailed analysis of this wet side of the function has never been performed, in contrast to the dry side of the Feddes-function (the part between h_3 and h_4) (Metselaar and de Jong van Lier, 2007). None of the procedures for root water uptake, including the Feddes-function, combine both plant physiological and soil physical processes to predict the reduction of root water uptake at insufficient soil aeration.

Feddes et al. (1978) already indicated that a fixed anaerobiosis point h_2 , identical for all environmental conditions, may be inappropriate, because pressure heads do not provide direct information on the aeration status of the soil. Alternative approximations of oxygen stress have been defined, like the gas filled porosity of the soil, ϕ_{gas} (Wesseling and van Wijk, 1957). This proxy might provide a better relationship between soil aeration and root oxygen stress, as soil aeration substantially depends on ϕ_{gas} (Hillel, 1980) and plant functioning appears to be well-correlated to this proxy (Dasberg and Bakker, 1970). Constant critical values for ϕ_{gas} have frequently been applied to represent oxygen stress (Barber et al., 2004; Leao et al., 2006), but constants are unlikely to be sufficient for any proxy. In fact, oxygen consumption of, and oxygen transport to plant roots depend on soil temperature, growth stage, soil texture and microbial activity (Hillel, 1980). Each of these variables should be considered simultaneously to determine the degree of oxygen stress accurately, but an accurate procedure does not seem to exist up to now. Such a procedure should

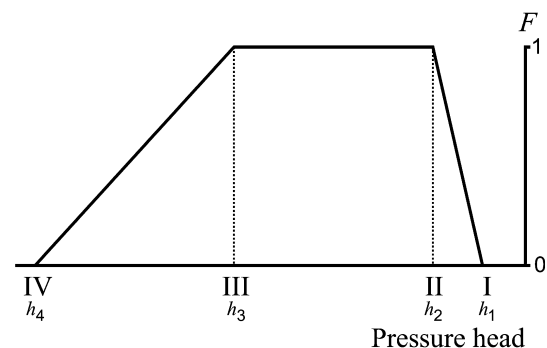


Figure 1 Sink term variable F as function of pressure head h according to Feddes et al. (1978). Root water uptake reduces linearly from III (h_3) to IV (h_4) due to moisture stress, as well as from the critical values II (h_2) and I (h_1), due to oxygen stress. In between II and III, root water uptake is optimal ($F = 1$).

combine two very different types of equations: (1) Oxygen consumption of plant roots described by plant physiological processes, focusing on the energy demand of plants (Cannell and Thornley, 2000), and (2) Oxygen transport to plant roots described by physical laws, focusing on the diffusion of oxygen through different media (e.g. Glinski and Stepniewski, 1985). These plant physiological and soil physical processes have to be considered simultaneously, as the oxygen transport (ad 1) is determined by oxygen consumption (ad 2) and vice versa.

In this paper we introduce such a procedure: we propose a model to compute plant oxygen stress based on the above mentioned processes. Through this model, we quantified the sensitivity of oxygen stress to various model parameters. Moreover, we calculated root water uptake reduction under the influence of oxygen stress. Finally, we argue why our model will lead to better predictions of root water uptake under oxygen stress than the Feddes-function.

Model description

General setup

The general model setup is visualized by Fig. 2. The main output parameter of our model is the minimum gas filled porosity of the soil ϕ_{gas_min} at which oxygen stress occurs (Fig. 2C). To calculate this parameter, we need to model the diffusion-driven transport of oxygen from the gas phase of the soil to root cells (oxygen diffusion at the micro-scale; Fig. 2A and B) and from the atmosphere to the gas phase of the soil (oxygen diffusion at the macro-scale; Fig. 2C and D) (De Willigen and Van Noordwijk, 1987). Diffusion fluxes, described by Fick’s law, are determined by: (a) oxygen consuming processes, (b) diffusivity, which depends on the medium through which diffusion takes place, (c) the concentration gradient, which depends on (d) the distance over which diffusion takes place. These aspects are different for

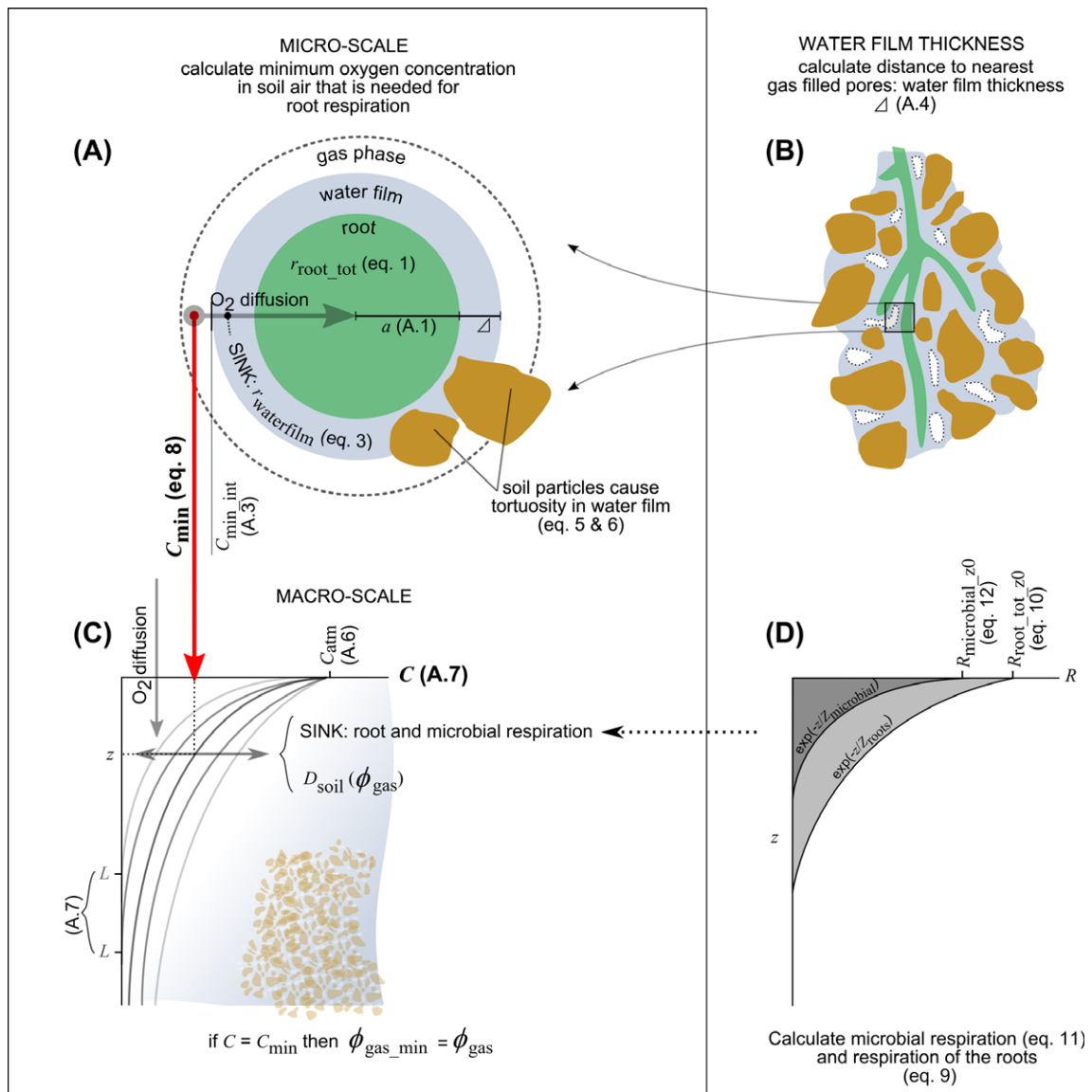


Figure 2 Scheme for the calculation of critical values for oxygen stress, based on both physiological and physical processes.

Table 1 Parameters that are involved in the diffusion processes for oxygen supply to plant roots

	Micro-scale (Fig. 2A and B)	Macro-scale (Fig. 2C and D)
Oxygen consuming processes	Root respiration ($r_{\text{root_tot}}$) Microbial respiration ($r_{\text{waterfilm}}$)	Root respiration ($R_{\text{root_tot}}$) Microbial respiration ($R_{\text{microbial}}$)
Diffusivity	Water-film ($D_{\text{waterfilm}}$) root tissue (D_{root})	Soil (D_{soil})
Gradient	[O ₂] gas phase soil (C_{min}) – [O ₂] center of root (0)	[O ₂] atmosphere (C_{atm}) – [O ₂] gas phase soil (C)
Distance	Thickness water-film (Δ) + root radius (a)	Soil surface to certain depth (z)

diffusion at the micro-scale and macro-scale (Table 1) and will be discussed in detail in sections “Calculation of C_{min} (diffusion at the micro-scale)” and “Calculation of C (diffusion at the macro-scale)” respectively.

Diffusion at the micro-scale (Fig. 2A and B) focuses on the minimum oxygen concentration in the gas phase of the soil (C_{min}), needed to meet the oxygen requirements of roots. We schematized roots as cylinders and assumed that the root zone has a uniform soil texture and temperature. Subsequently, C_{min} was calculated based on oxygen consumption and diffusion pathway through a root cross-section (Fig. 2A). Two temperature dependent oxygen consuming processes occur in the root zone: respiration of roots (needed for both maintenance and root growth) and microbial respiration in the water-film surrounding the roots. The water-film is a thin layer of soil moisture that covers soil particles and plant roots (Fig. 2B). Oxygen that diffuses from the gas phase of the soil to the root passes this water-film. Because the diffusivity of oxygen in water is 10^4 times lower than that in free air (Stumm and Morgan, 1996), this water layer can be a serious barrier for oxygen diffusion to plant roots (Armstrong and Beckett, 1985; De Willigen and Van Noordwijk, 1984).

Diffusion at the macro-scale (Fig. 2C and D) focuses on oxygen transport from the atmosphere through the soil to the gas phase surrounding the roots. Root respiration and microbial respiration are sink terms, eliminating oxygen from the gas phase of the soil. We assumed that both volumetric root density and microbial respiration rate decrease exponentially with depth (Campbell, 1985 fide Cook, 1995). As a result, oxygen concentration C decreases with depth z in the soil profile. The diffusivity of the soil typically controls soil aeration and varies with soil type and gas filled porosity ϕ_{gas} (Buckingham, 1904; Moldrup et al., 2000).

In our model, both scales of diffusion were linked by iteratively adjusting ϕ_{gas} until C (macro-scale) equaled C_{min} . This resulted in the minimum gas filled porosity of the soil, $\phi_{\text{gas_min}}$, needed to meet the oxygen requirements of plant roots at soil depth z . $\phi_{\text{gas_min}}$ is a threshold for oxygen stress and depends on both abiotic and biotic conditions, like soil texture, soil temperature, growth stage and microbial activity.

Parameterization

All model parameters are given in Table 2. We used the model to calculate $\phi_{\text{gas_min}}$ for different soil physical properties derived for sandy, loamy and clayey soils (Table 3, Fig. 3). All plant characteristics used for calculating $\phi_{\text{gas_min}}$

(see also Appendix A.1) were mean values, taken from literature, for a temperate terrestrial natural grassland. All parameter values were derived from independent sources, and thus were not optimized to improve model results. Other parameter values than chosen here, e.g. for other vegetations, may be used to calculate $\phi_{\text{gas_min}}$.

Calculation of C_{min} (diffusion at the micro-scale)

Oxygen consuming processes at the micro-scale

The calculation of root respiration is based on the growth-and-maintenance-respiration paradigm, which involves both empirical studies and theoretical principles (Amthor, 2000). Despite the partly empirical basis of the equations, they are commonly used in plant physiological modeling.

Applying this approach, total respiration of a cylindrical root $r_{\text{root_tot}}$ ($\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$) was calculated from the root respiration at a reference temperature $r_{\text{root_tot_ref}}$ ($\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$) correcting for differences in soil temperature T_{soil} (K) (Amthor, 2000):

$$r_{\text{root_tot}} = r_{\text{root_tot_ref}} \cdot Q_{10_{\text{root}}}^{(T_{\text{soil}} - T_{\text{ref}})/10} \quad (1)$$

where $Q_{10_{\text{root}}}$ is the relative increase in $r_{\text{root_tot}}$ at a temperature increase of 10 °C (–) (Atlas and Bartha, 1987). Q_{10} is a widely accepted empirical measure to describe the sensitivity of plant physiological processes to temperature (Lloyd and Taylor, 1994).

$r_{\text{root_tot_ref}}$ is the sum of reference maintenance respiration and reference growth respiration. Oxygen is always used first for maintenance, and only if oxygen availability allows, additional oxygen is used for growth respiration. Reference maintenance respiration $r_{\text{root_m_ref}}$ ($\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$) is described as (Amthor, 2000):

$$r_{\text{root_m_ref}} = k_m \cdot w \quad (2)$$

where k_m is the empirical maintenance coefficient of roots ($\text{kg O}_2 \text{ kg}^{-1} \text{ root d}^{-1}$) and w the specific root mass ($\text{kg root m}^{-1} \text{ root}$). In our approach, total respiration is taken relative to maintenance respiration. This ratio is depicted as η (–), and it is assumed that $\eta = \eta_{\text{potential}} = 5$ at optimal oxygen availability (Penning de Vries et al., 1979). ϕ_{gas} for $\eta = 1$ and ϕ_{gas} for $\eta = \eta_{\text{potential}}$ correspond to the points I (h_1) and II (h_2) in the Feddes-function (Fig. 1), respectively.

Microbial respiration in the water-film $r_{\text{waterfilm}}$ ($\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$) was assumed to decrease exponentially with depth z (m below soil surface) (Campbell, 1985 fide Cook, 1995):

Table 2 Input parameters and calculated parameters (including standard deviations) used in the model

Symbol	Unit	Description	Value
Input parameters			
k_m	—	Maintenance coefficient	0.016 ± 0.008 (Kroes et al., 2008)
M	—	Van Genuchten parameter M	Table 3
M_{O_2}	kg mol ⁻¹	Molar mass of dioxygen	0.032
N	—	Van Genuchten parameter N	Table 3
p	Pa	atmospheric pressure	1e5
Q_{10_root}	—	Relative increase in root respiration rate at a temperature increase of 10 °C	2.0 (Amthor, 2000)
$Q_{10_microbial}$	—	Relative increase in microbial respiration rate at a temperature increase of 10 °C	2.8 (Fierer et al., 2006)
R	m ³ Pa K ⁻¹ mol ⁻¹	Universal gas constant	8.314427
S	kg root m ⁻³ root	Specific weight of non-airfilled root tissue	1.0e3 (De Willigen and Van Noordwijk, 1987)
SRL	m root kg ⁻¹ root	Specific root length	3.8 ± 1.6e5 (De Willigen and Van Noordwijk, 1987)
T_{air}	K	Air temperature	273–303
T_{soil}	K	Soil temperature	273–303
T_{ref}	K	Reference temperature	298
$var(a)$	m ²	Variance of a	4.175e-10 (De Willigen and Van Noordwijk, 1987)
W	kg root m ⁻³ soil	Dry weight of bulk roots at $z = 0$	0.785 ± 0.385 (Jackson et al., 1996)
Y	—	Dry matter content of roots	0.07 (De Willigen and Van Noordwijk, 1987)
z	m	Depth	0.0–0.5
$Z_{microbial}$	m	Shape factor for exponential decrease of microbial respiration with depth	0.3 (Campbell, 1985 fide Cook and Knight, 2003)
Z_{root}	m	Shape factor for exponential decrease of root respiration with depth	0.127 ± 0.013 (Jackson et al., 1996)
α	1/Pa	Van Genuchten parameter α	Table 3
β	kg O ₂ kg ⁻¹ C d ⁻¹	Vegetation dependent respiration rate	2.258 ± 1.085e-4 (Fierer et al., 2006)
ε_{org}	%	Organic matter content of the soil	0.0–15.0
η	—	respiration factor	1–5 (Penning de Vries et al., 1979)
θ_{res}	—	Residual water content	Table 3
θ_{sat}	—	Saturated water content	Table 3
ρ_{soil}	kg soil m ⁻³ soil	Soil density	Table 3
τ_{root}	—	Tortuosity of the root tissue	0.4
ϕ_{root}	—	Air filled root porosity	0.05 (De Willigen and Van Noordwijk, 1987)
Calculated parameters			
a	m	Root radius	
A	m ²	Area of a cross-section of water-film	
b	—	Campbell soil water retention parameter	
C	kg O ₂ m ⁻³ soil air	Oxygen concentration in the gas phase of the soil	
C_{atm}	kg O ₂ m ⁻³ air	Oxygen concentration in the atmosphere	
C_{min}	kg O ₂ m ⁻³ root	minimum oxygen concentration in the gas phase of the soil	
C_{min_int}	kg O ₂ m ⁻³ root	Minimum oxygen concentration at the interface of the water-film and the gas phase of the soil	
D_0	m ² d ⁻¹	Diffusivity of oxygen in free air	
D_{root}	m ² d ⁻¹	Diffusivity of the root	
D_{soil}	m ² d ⁻¹	Mean diffusivity of the soil	
D_{water}	m ² d ⁻¹	Diffusivity of water	
$D_{waterfilm}$	m ² d ⁻¹	Diffusivity of water-film	

(continued on next page)

Table 2 (continued)

Symbol	Unit	Description
f_{φ}	—	Reduction factor for microbial respiration through moisture
F	—	Sink term variable
h	cm	Soil water pressure head
L	m	Depth where $C = 0$
n	m^{-2} soil	Length density of gas filled pores
$R_{\text{microbial}}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	Volumetric microbial respiration of the soil
$R_{\text{microbial}_z0}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	Volumetric microbial respiration of the soil at $z = 0$
$r_{\text{root}_m\text{ref}}$	$\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$	Reference maintenance respiration per unit length of root
$R_{\text{root}_m z0\text{ref}}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	volumetric reference root maintenance respiration at $z = 0$
$R_{\text{root}_\text{tot}}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	Volumetric total root respiration
$r_{\text{root}_\text{tot}}$	$\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$	Total respiration per unit length of root
$r_{\text{root}_\text{tot}_\text{ref}}$	$\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$	Reference total respiration per unit length of root
$R_{\text{root}_\text{tot}_z0}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	Volumetric total root respiration at $z = 0$
$R_{\text{root}_\text{tot}_z0\text{ref}}$	$\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$	Volumetric reference total root respiration at $z = 0$
$r_{\text{waterfilm}}$	$\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$	Microbial respiration rate in water-film
$r_{\text{waterfilm}_z0}$	$\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$	Microbial respiration in water-film at $z = 0$
w	$\text{kg root m}^{-1} \text{ root}$	Specific root mass
α_B	$\text{m}^3 \text{ gas m}^{-3} \text{ liquid}$	Bunsen solubility coefficient for oxygen
δ	—	Ratio of rhizosphere (water-film) respiration to the total root respiration
Δ	m	Thickness of water-film
ϵ_{sand}	%	Sand content of the soil
θ	—	Water content
λ	—	Ratio of D_{root} and $D_{\text{waterfilm}}$
σ	N m^{-1}	Surface tension of water
μ	$\text{kg C m}^{-3} \text{ soil}$	Organic carbon content of the soil
ϕ_{gas}	—	Gas filled porosity of the soil
$\phi_{\text{gas}_\text{min}}$	—	Minimum gas filled porosity that is needed to meet the oxygen requirements of the roots
$\phi_{\text{waterfilm}}$	$\text{m}^3 \text{ soil particles m}^{-3} \text{ water-film}$	Porosity of the water-film
ϕ_{gas_100}	—	Gas filled porosity at $h = 100$ cm
ϕ_{total}	—	Total porosity of the soil
ϕ	Pa	Matric potential of soil moisture
ϕ_{sat}	Pa	Saturated matric potential

$$r_{\text{waterfilm}} = r_{\text{waterfilm}_z0} \cdot \exp(-z/Z_{\text{microbial}}) \quad (3)$$

where $r_{\text{waterfilm}_z0}$ represents the microbial respiration rate in the water-film ($\text{kg O}_2 \text{ m}^{-1} \text{ root d}^{-1}$) at the soil surface. $Z_{\text{microbial}}$ is a shape parameter that empirically describes the decrease of organic resources for microbial respiration with depth z . Microbial respiration was calculated as an empirical function of T_{soil} (K), organic carbon content of the soil μ ($\text{kg C m}^{-3} \text{ soil}$) (Appendix A.2) and vegetation dependent respiration rate β ($\text{kg O}_2 \text{ kg}^{-1} \text{ C d}^{-1}$) (Arora, 2003):

$$r_{\text{waterfilm}_z0} = 0.5 \cdot (\mu \cdot A) \cdot \beta \cdot Q_{10_{\text{microbial}}}^{(T_{\text{soil}} - T_{\text{ref}})/10} \quad (4)$$

with $Q_{10_{\text{microbial}}}$ the relative increase in $r_{\text{waterfilm}_z0}$ at a temperature increase of 10°C (—) (Atlas and Bartha,

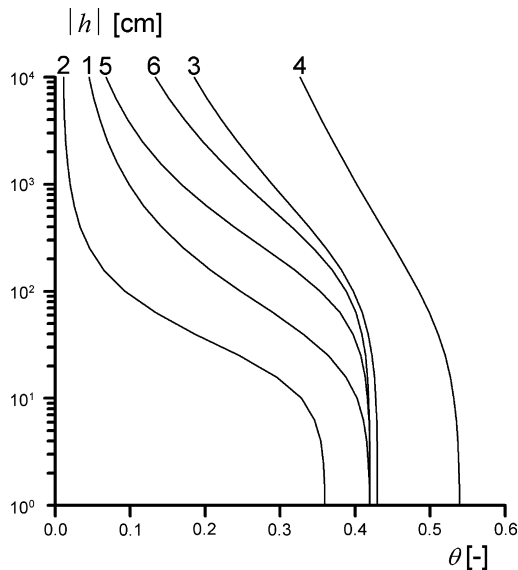
1987). A is the area of a cross-section of the cylindrical water-film (m^2).

Diffusivity at the micro-scale

The diffusivity for oxygen in the water-film $D_{\text{waterfilm}}$ ($\text{m}^2 \text{ d}^{-1}$) was derived from the diffusivity for oxygen in water D_{water} ($\text{m}^2 \text{ d}^{-1}$) and a correction for the tortuosity of the water-film. As the thickness of the water-film equals the distance from the root surface to the nearest gas filled pores (see section "Distance at the micro-scale"), the water-film can be regarded as a saturated soil. Therefore, the calculation of the diffusivity for oxygen in the water-film is equivalent to that of the diffusivity in a saturated soil, as described by Millington and Quirk (1961):

Table 3 Soil types and soil physical characteristics (Wösten et al., 2001) that were used in the calculation of critical values for oxygen stress

No.	Soil type	θ_{res} (-)	θ_{sat} (-)	α (1/Pa)	N ($M = 1 - 1/N$) (-)
1	Moderately loamy, very fine sand	0.02	0.42	2.76e-4	1.491
2	Course sand	0.01	0.36	4.52e-4	1.933
3	Light clay	0.01	0.43	6.4e-4	1.210
4	Heavy clay	0.01	0.54	2.39e-4	1.094
5	Sandy loam	0.01	0.42	8.4e-4	1.441
6	Silty loam	0.01	0.42	5.1e-4	1.305

**Figure 3** Soil water retention curves (Wösten et al., 2001) for the soil types that were used in the calculation of critical values for oxygen stress. The numbers in the retention curves correspond to the soil types and the soil physical characteristics in Table 3.

$$D_{\text{waterfilm}} = D_{\text{water}} \cdot \phi_{\text{waterfilm}}^{4/3} \quad (5)$$

where $\phi_{\text{waterfilm}}$ is called the 'porosity of the water-film' ($\text{m}^3 \text{water m}^{-3} \text{water-film}$) defined as the ratio between the soil water content and the volume of the liquid and solid phase (Currie, 1965 fide Simojoki, 2000):

$$\phi_{\text{waterfilm}} = (\phi_{\text{total}} - \phi_{\text{gas}}) / (1 - \phi_{\text{gas}}) \quad (6)$$

with ϕ_{total} the total porosity of the soil and ϕ_{gas} the gas filled porosity of the soil.

The diffusivity for oxygen in the plant root D_{root} was derived from D_{water} , assuming that the sensitivity of D_{root} to temperature equals that of D_{water} (Langø et al., 1996), and a correction for the tortuosity of root tissues τ_{root} (-):

$$D_{\text{root}} = \tau_{\text{root}} \cdot D_{\text{water}} \quad (7)$$

By scaling a published reference value of D_{root} for a terrestrial grassland species at $T_{\text{soil}} = 293$ K (Van Noordwijk and De Willigen, 1984) to D_{water} , we obtained $\tau_{\text{root}} = 0.4$.

Concentration gradient at the micro-scale

A steady-state equation for the distribution of the concentration of oxygen in the water-film and the root (De Willigen

and Van Noordwijk, 1984) was used to calculate $C_{\text{min_int}}$ (Appendix A.3). $C_{\text{min_int}}$ ($\text{kg O}_2 \text{m}^{-3} \text{root}$) represents the oxygen concentration at the interface of the water-film and the gas phase of the soil, that is required to ensure sufficient oxygen supply for $r_{\text{root_tot}}$ to all cells in the root (De Willigen and Van Noordwijk, 1987). The oxygen concentration at the outer edge of the water-film $C_{\text{min_int}}$ and the gas phase of the soil C_{min} were considered to be in equilibrium, thus:

$$C_{\text{min}} = C_{\text{min_int}} / \alpha_B \quad (8)$$

where α_B is the Bunsen solubility coefficient for oxygen ($\text{m}^3 \text{gas m}^{-3} \text{liquid}$) (Langø et al., 1996).

Distance at the micro-scale

The thickness of the water-film Δ (m), i.e. the distance from the root surface to the nearest gas filled pores, was calculated according to Simojoki (2000) (Appendix A.4). Root radius a (m) was calculated according to De Willigen and Van Noordwijk (1987) (Appendix A.1).

Calculation of C (diffusion at the macro-scale)

Oxygen consuming processes at the macro-scale

The calculation of the total root respiration of the bulk roots at $z = 0$ m $R_{\text{root_tot_z0}}$ ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$) was similar to the procedure for a cylindrical root (Eq. (1)). The only difference is that respiration rates are considered per volume soil ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$), instead of per meter root ($\text{kg O}_2 \text{m}^{-1} \text{root d}^{-1}$). $R_{\text{root_tot}}$ was assumed to decrease exponentially with z , based on the decrease of root dry weight with depth (Campbell, 1985 fide Cook, 1995):

$$R_{\text{root_tot}} = R_{\text{root_tot_z0}} \cdot \exp(-z/Z_{\text{root}}) \quad (9)$$

where Z_{root} is an empirical shape factor and $R_{\text{root_tot_z0}}$ is the total root respiration at depth $z = 0$ m ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$):

$$R_{\text{root_tot_z0}} = R_{\text{root_tot_z0_ref}} \cdot Q_{10_{\text{root}}}^{(T_{\text{soil}} - T_{\text{ref}})/10} \quad (10)$$

and the reference total root respiration at $z = 0$ $R_{\text{root_tot_z0_ref}}$ ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$) as defined in section "Oxygen consuming processes at the micro-scale", but using W (substituting w , Eq. (2)) as the dry weight of bulk roots at $z = 0$ m ($\text{kg root m}^{-3} \text{soil}$).

The calculation of the microbial respiration in the bulk soil $R_{\text{microbial}}$ ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$) was also similar to that of $r_{\text{waterfilm}}$ (Eq. (3)). The differences are that volumetric respiration rates, i.e. ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$), and unsaturated conditions are considered here:

$$R_{\text{microbial}} = R_{\text{microbial_z0}} \cdot \exp(-z/Z_{\text{microbial}}) \quad (11)$$

with the microbial respiration at $z = 0$ m $R_{\text{microbial}_z0}$ ($\text{kg O}_2 \text{m}^{-3} \text{soil d}^{-1}$):

$$R_{\text{microbial}_z0} = f_{\varphi} \cdot \mu \cdot \beta \cdot Q_{10_{\text{microbial}}}^{(T_{\text{soil}} - T_{\text{ref}})/10} \quad (12)$$

with f_{φ} a reduction factor for soil moisture (–) (Appendix A.5).

Diffusivity at the macro-scale

The mean diffusivity of soils D_{soil} ($\text{m}^2 \text{d}^{-1}$) was calculated from soil water characteristics, and thus pore size distributions, according to Moldrup et al. (2000):

$$D_{\text{soil}} = D_0 \cdot (2 \cdot \phi_{\text{gas}_100}^3 + 0.04 \cdot \phi_{\text{gas}_100}) \cdot (\phi_{\text{gas}} / \phi_{\text{gas}_100})^{2+3/b} \quad (13)$$

where D_0 is the diffusion coefficient for oxygen in free air ($\text{m}^2 \text{d}^{-1}$), ϕ_{gas_100} is the gas filled porosity at a soil water pressure head $h = -100$ cm (–) and b = the Campbell soil water retention parameter (Campbell, 1974). The b -value can be determined as the slope of the soil water retention curve in a log–log plot ($\log[\theta]$ vs. $\log[-h]$), which means that the soil water retention characteristics have to be known at least at two h 's. Moldrup et al. (2000) propose to take: $b = (\log[500] - \log[100]) / (\theta_{h=-100\text{cm}} - \theta_{h=-500\text{cm}})$. Moldrup et al. (2000) showed that the inclusion of soil water characteristics in the calculation of D_{soil} represents the measured mean D_{soil} much better than previous models that only considered the gas filled porosity (ϕ_{gas}) and the total porosity (ϕ_{total}) of the soil (e.g. Millington and Quirk, 1961). Such models highly underestimate D_{soil} for low ϕ_{gas} (Moldrup et al., 2000).

Concentration gradient at the macro-scale

The concentration gradient at the macro-scale was determined by the oxygen concentration in the atmosphere C_{atm} ($\text{kg O}_2 \text{m}^{-3} \text{air}$) and the oxygen concentration C ($\text{kg O}_2 \text{m}^{-3} \text{soil air}$) in the soil at a certain depth z . C_{atm} was calculated according the general gas law, assuming 21% of oxygen in the atmosphere (Appendix A.6). An analytical solution for $C(z)$, considering the exponential decrease of both root and microbial respiration with depth, is given by Cook (1995). To increase the flexibility of our model, we considered, unlike Cook (1995), root and microbial respiration as two separate sink terms with specific exponential decreases, leading to slightly adapted equations (Fig. 2D and Appendix A.7).

Distance at the macro-scale

The distance over which diffusion takes place equals depth z (m below soil surface) at which the oxygen concentration is calculated.

The relation between oxygen stress and water uptake

Our model computes $\phi_{\text{gas}_\text{min}}$ as a function of the oxygen demand of plant roots for root respiration. However, it is also possible to compute root water uptake as function of $\phi_{\text{gas}_\text{min}}$. The latter approach was used to evaluate the relation between oxygen stress and root water uptake. To do so, we assumed that root water uptake is proportional to growth respiration. There are several arguments that support this assumption.

Root water uptake occurs by hydrostatic forces (passive transport) and by the metabolic activity of root cells (active transport). Stomata represent the highest resistance to water flow (Ehlers and Goss, 2003; Katul et al., 2003). If stomata are fully opened, root water uptake is optimal ($F = 1$) and dominated by hydrostatic forces. At fully open stomata, potential photosynthesis is achieved and oxygen is needed for both maintenance and growth respiration. Potential root water uptake is thus only possible as long as there is no oxygen stress. Oxygen stress induces stomatal closure (e.g. Glinski and Stępniewski, 1985; Kramer, 1951). At complete stomatal closure, the actual transpiration and photosynthesis approach zero ($F = 0$). In that case, oxygen is solely used for maintenance respiration.

Between the limits $F = 1$ and $F = 0$, we assume the reduction of root water uptake to be directly proportional to the reduction in root respiration: Kamaluddin and Zwiazek (2001) demonstrated, by inhibition of the metabolism of the roots, that there is a positive correlation between root respiration and water uptake. This implies a gradual decrease of root water uptake with increased oxygen stress.

Model analysis

Sensitivity of $\phi_{\text{gas}_\text{min}}$

ϕ_{gas} was iteratively adjusted between 10^{-8} (~ 0) and ϕ_{total} , until the convergence criterion $\text{abs}(C_{\text{min}} - C) < 10^{-4} \text{ kg m}^{-3}$ was met. This ϕ_{gas} corresponds to $\phi_{\text{gas}_\text{min}}$ (Fig. 2A and C). Together with adjusting ϕ_{gas} , the parameters depending on ϕ_{gas} (Δ , $R_{\text{microbial}_z0}$ and D_{soil} , and thus both C_{min} and C), were recalculated.

After numerical verification of our model, we analyzed the validity of uniform critical values h_1 and h_2 for oxygen stress (Fig. 1). A sensitivity analysis for $\phi_{\text{gas}_\text{min}}$, and here-with h , was performed for different abiotic conditions, relevant for The Netherlands. We distinguished different soil types (Table 3, Fig. 3), temperatures ($T_{\text{soil}} = T_{\text{air}} = 273 - 303$ K), organic matter contents ($\epsilon_{\text{org}} = 0.0 - 15.0\%$), depths ($z = 0.0 - 0.5$ m) and oxygen requirements ($1 \leq \eta \leq 5$).

Secondly, we performed a Monte Carlo analysis to study the sensitivity of $\phi_{\text{gas}_\text{min}}$ to plant characteristics. Plant characteristics were randomly extracted from normal distributions, defined by average values and standard deviations (Table 2). $\phi_{\text{gas}_\text{min}}$ was calculated for each combination of abiotic conditions (soil type, T_{soil} , ϵ_{org} and z) and for thousands of extractions from the normal distributions of plant characteristics. Monte Carlo analysis was performed both for $\eta = 1$ and $\eta = 5$. $\phi_{\text{gas}_\text{min}}$ values were normalized to the average $\phi_{\text{gas}_\text{min}}$ across all simulations. Linear regression was used to analyze the sensitivity of normalized $\phi_{\text{gas}_\text{min}}$ to each plant characteristic. Variation in the $\phi_{\text{gas}_\text{min}}$ values around each regression line, caused by variation in all parameters other than the plant characteristic on the x-axis, was visualized by regression quantiles (Koenker, 2007).

Sensitivity of F

We used the model to calculate F (Fig. 1) as function of $\phi_{\text{gas}_\text{min}}$ (see section ‘‘The relation between oxygen stress and water uptake’’). η was iteratively adjusted between

10^{-4} (~ 0) and $\eta_{\text{potential}}$, until $\text{abs}(C_{\text{min}} - C) < 10^{-4} \text{ kg m}^{-3}$. $\eta = 1$ and $\eta = \eta_{\text{potential}}$ correspond to $F = 0$ and $F = 1$, respectively. Together with adjusting η , the parameters $r_{\text{root_tot}}$ and $R_{\text{root_tot_z0}}$, and thus both C_{min} and C , were recalculated. Since $\phi_{\text{gas_min}}$ is related to h – via soil porosity and the water retention curve – this enabled us to compare F from our model with F from the reduction function of Feddes et al. (1978).

Results

Sensitivity of $\phi_{\text{gas_min}}$ and F to environmental parameters

The minimum gas filled porosity $\phi_{\text{gas_min}}$, and herewith the soil water pressure head h corresponding to oxygen stress, was especially sensitive to the abiotic parameters soil temperature T_{soil} and depth z (Fig. 4). $\phi_{\text{gas_min}}$ was hardly sensitive to soil organic matter content ϵ_{org} . This sensitivity pattern held for all investigated six soil types, although $\phi_{\text{gas_min}}$ differed considerably between soil types.

The Feddes-function uses uniform values h_1 and h_2 for a specific crop type or plant species. Values of $h_1 = -10$ cm and $h_2 = -25$ cm are commonly used for grasslands (Feddes and Raats, 2004; Kroes et al., 2008; Wesseling, 1991). In all states tested, oxygen stress started at more negative h (drier) conditions, than these standard values (Fig. 4). The differences between the calculated reduction functions are considerable among the various soil types (Fig. 5). $\phi_{\text{gas_min}}$ was larger in sandy soils than in soils that contain clay particles, as could be expected (Håkansson and Lipiec, 2000; Pierce et al., 1983). Clayey soils are well structured, which provides connected gas filled pores through which diffusion occurs. Sandy soils with high water contents consist of isolated gas filled pores that cannot contribute to the oxygen diffusion pathway (Horn et al., 1994). Especially for clayey and loamy soils, the critical h -values of Wesseling (1991) corresponded to extremely low ϕ_{gas} -values that are unlikely to be sufficient (< 0.01 , see Figs. 3 and 5 and Table 3) for the oxygen requirements of roots. Unfortunately, in spite of all our efforts we were unable to discover how Wesseling (1991) derived the h -values.

Analysis of our model showed that transpiration reduction differed strongly between soil types (Fig. 5), but that within a specific soil type, F mainly depends on T_{soil} , z and ϕ_{gas} (Figs. 4 and 6). The reduction was highly nonlinear with z and the influence of temperature was considerable (Fig. 6), which means that F (Fig. 5) shifts to a different $\phi_{\text{gas_min}}$ (and h) upon changes in T_{soil} and z . Like the original Feddes function (Feddes et al., 1978), the shape F as function of h (Fig. 5b) was close to linear.

Sensitivity of $\phi_{\text{gas_min}}$ to plant characteristics

$\phi_{\text{gas_min}}$ appeared to be especially sensitive to plant characteristics W and k_m and hardly to SRL , β and Z_{root} (Fig. 7). The differences in sensitivity to W vs. SRL imply that the characteristics of a single cylindrical root (w and a , calculated from SRL , Appendix A.1), have less influence on $\phi_{\text{gas_min}}$ than the characteristics of the bulk roots. This indicates that diffusion processes at the micro-scale were less influential than those at the macro-scale. This corresponds to our finding that in the diffusion at the macro-scale, only a small change in ϕ_{gas} is needed to provide a large change in C . The sensitivity of $\phi_{\text{gas_min}}$ to the maintenance coefficient k_m can be problematic for some model applications, because k_m is an empirical parameter that is difficult to acquire accurately (Cannell and Thornley, 2000).

Discussion

Progress obtained in the simulation of oxygen stress

In this paper, we introduced a process-based model to simulate the minimum gas filled porosity $\phi_{\text{gas_min}}$, needed to provide plant roots with just sufficient oxygen for root maintenance and growth respiration. Both the oxygen demand of plant roots and soil microbes and the oxygen transport from the atmosphere, through the soil and to the roots were incorporated. Our model is based on important processes involved in the diffusion processes at the micro-scale (described by e.g. Armstrong and Beckett, 1985; De Willigen and Van Noordwijk, 1984; Glinski and Stępniewski, 1985; Lemon and Wiegand, 1962) and macro-scale (described by

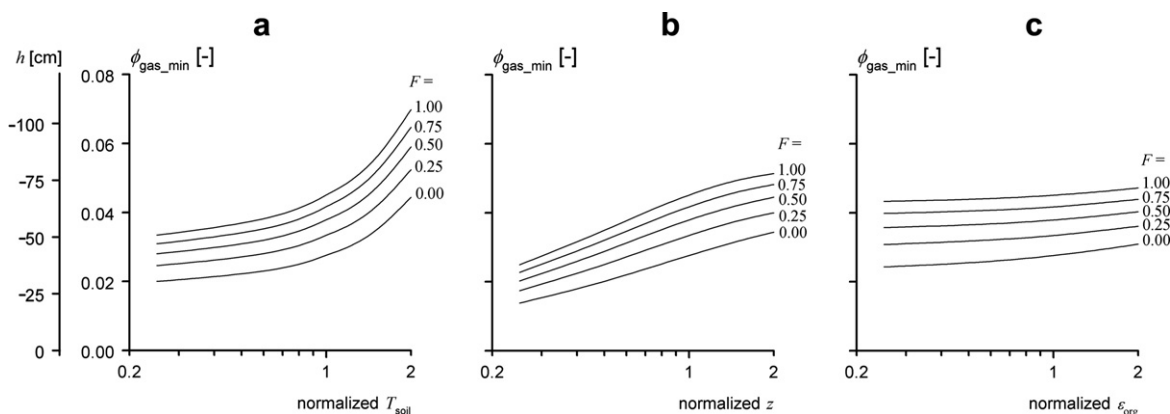


Figure 4 Sensitivity of $\phi_{\text{gas_min}}$ and h to (a) T_{soil} , (b) z and (c) ϵ_{org} at different respiration rates (varying from $\eta = 1$ ($F = 0$), to $\eta = 5$ ($F = 1$)) for a temperate terrestrial grassland (Table 2) on sandy loam (soil type = 5, Table 3). T_{soil} , ϵ_{org} and z were normalized around the reference values 15 °C (288 K), 7.5% and 0.25 m, respectively. For each analysis, only one of the abiotic parameters was varied, while keeping the other parameters at their reference values. Other investigated soil types show similar sensitivities.

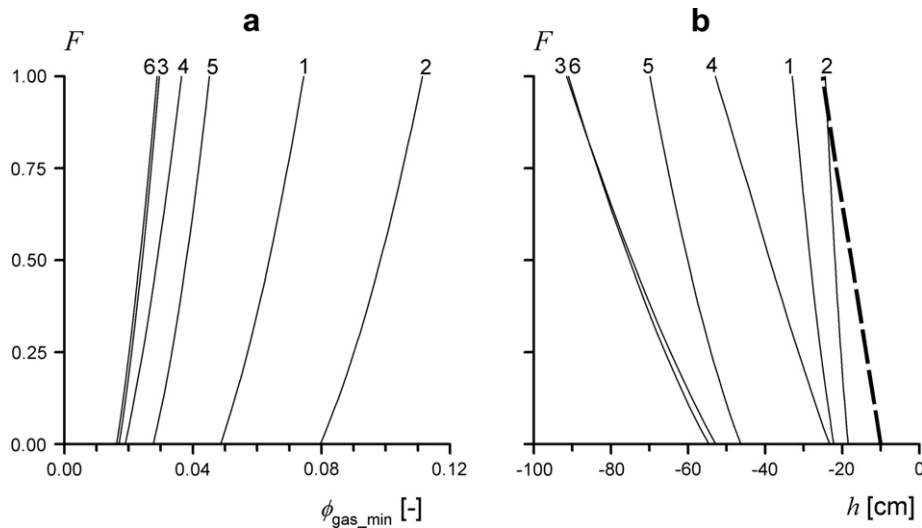


Figure 5 Sink term variable F as function of both soil type (Table 3) and (a) $\phi_{\text{gas_min}}$ and (b) h . $T_{\text{soil}} = 288$ K, $\epsilon_{\text{org}} = 7.5\%$, $z = 0.25$ m and average reference vegetation characteristics (Table 2). The dotted line in (b) represents the function by Feddes et al. (1978). The reduction functions are only valid for the very specific parameter values chosen here. For each of the soil types, the values for $\phi_{\text{gas_min}}$ and thus h change with e.g. T_{soil} and z .

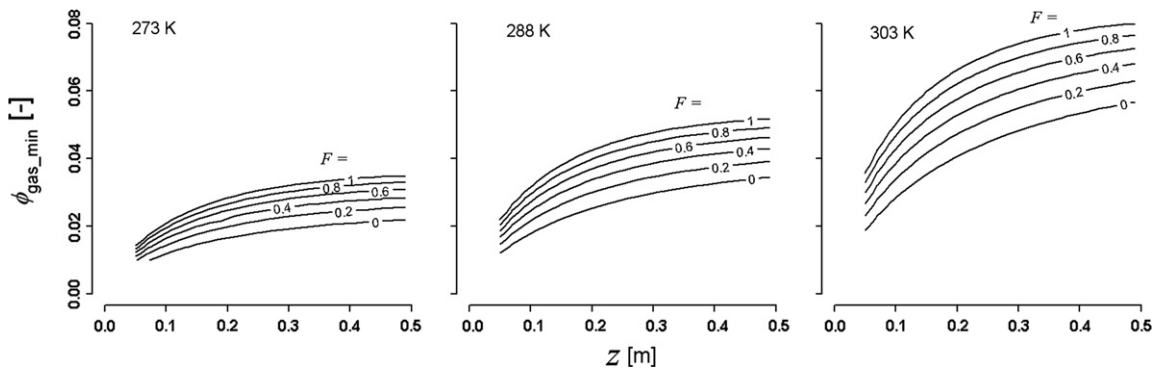


Figure 6 Contour plots of F as function of ϕ_{gas} and z for three temperatures ($T_{\text{soil}} =$ (a) 273 K, (b) 288 K and (c) 303 K) and $\epsilon_{\text{org}} = 7.5\%$; $T_{\text{soil}} = T_{\text{air}}$. Only the results for a sandy loam (soil type = 5, Table 3) are presented here, but the trend holds for all investigated soil types. The range in F -values corresponds to those of the y-axis in Fig. 5a.

e.g. Cook, 1995; Glinski and Stępniewski, 1985; Jones and Or, 1998; Kalita, 1999). So far, only one model considered diffusion at both scales (Cook and Knight, 2003). We combined the most appropriate equations involved in each of the diffusion processes, and extended and improved existing calculations where necessary.

Important improvements incorporated in our model are, first of all, to model microbial respiration in dependency of gas filled porosity ϕ_{gas} of the soil, and thus on water content. Overestimation of oxygen concentrations and $\phi_{\text{gas_min}}$ by too high microbial respiration rates (Cook and Knight, 2003; Kalita, 1999) is thus avoided. Second, we considered root and microbial respiration as two separate processes, instead of combining them (Cook, 1995; Glinski and Stępniewski, 1985; Jones and Or, 1998; Kalita, 1999). This has the advantage that the model has more flexibility in incorporating differences in depth profiles between root and microbial respiration. Third, the thickness of the water-film that covers plant roots and through which oxygen diffusion

takes place, was calculated as function of ϕ_{gas} and not taken as a fixed value (Armstrong and Beckett, 1985; Cook and Knight, 2003; Glinski and Stępniewski, 1985). Fourth, the microbial respiration within the water-film was considered instead of ignored (Cook and Knight, 2003; Glinski and Stępniewski, 1985; Lemon and Wiegand, 1962; Simojoki, 2000). Fifth, our calculation of the soil diffusivity D_{soil} on the basis of the soil water retention curve gives a better representation of D_{soil} at low ϕ_{gas} than the method of Millington and Quirk (1961) (Cook and Knight, 2003; Glinski and Stępniewski, 1985; Jones and Or, 1998). The method of Millington and Quirk (1961) is solely based on ϕ_{gas} , irrespective of soil type, and on total soil porosity ϕ_{total} . Moldrup et al. (2000) proved that the method of Millington and Quirk (1961) underestimates D_{soil} at low ϕ_{gas} , which results in an overestimation of $\phi_{\text{gas_min}}$.

All in all, we improved the descriptions of relevant processes and parameters and considered them simultaneously to calculate representative values for $\phi_{\text{gas_min}}$ accurately.

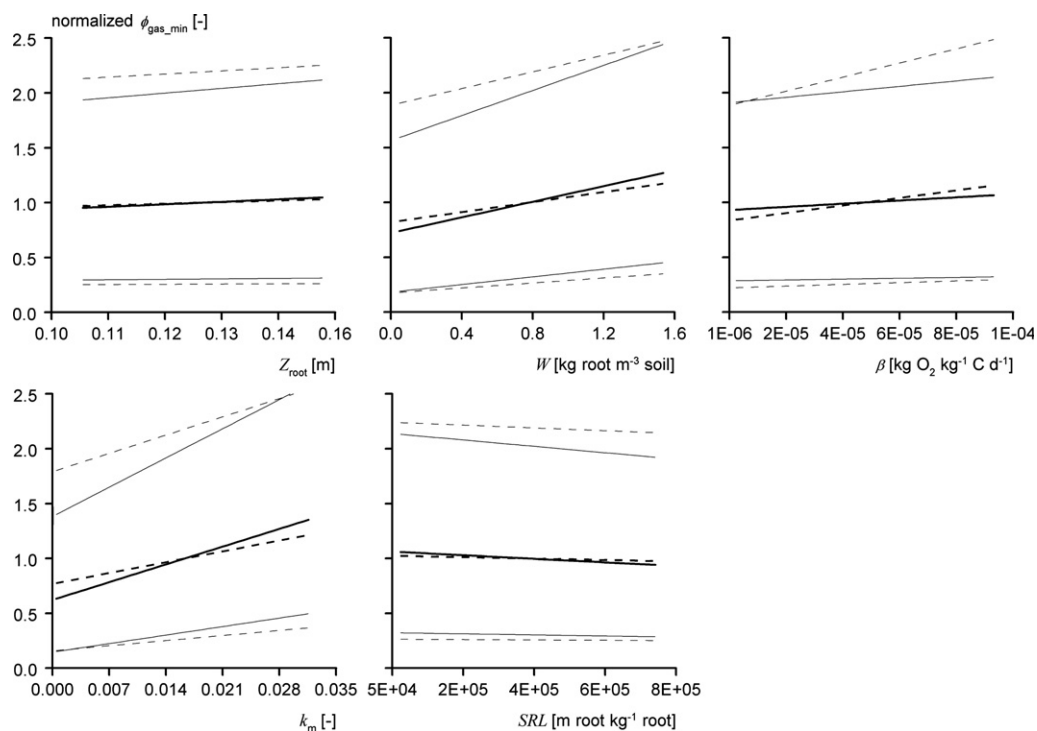


Figure 7 Sensitivity of $\phi_{\text{gas_min}}$ to plant characteristics of the reference plant species (Table 2). $\phi_{\text{gas_min}}$ is normalized around the mean $\phi_{\text{gas_min}}$ of all model runs. Monte Carlo analysis was performed for $\eta = 1$ (dotted lines) and $\eta = 5$ (solid lines). The slopes of the black lines indicate the effect on $\phi_{\text{gas_min}}$ of the parameter on the x-axis. The grey lines represent the 10 and 90% regression quantiles (Koenker, 2007). This bandwidth is caused by all varied parameters (abiotic and plant characteristics) other than the parameter on the x-axis.

Thus, we avoided the structural overestimation of $\phi_{\text{gas_min}}$ as happened in Cook and Knight (2003). Our model enabled us to simulate the variation in $\phi_{\text{gas_min}}$ resulting from differences in both abiotic and biotic conditions.

Constant vs. process-based critical measures for oxygen stress

In the literature, constant critical values for $\phi_{\text{gas_min}}$ have been applied to represent root oxygen stress (e.g. Barber et al., 2004; Leao et al., 2006). We demonstrated, however, that $\phi_{\text{gas_min}}$ depends on a number of environmental parameters, especially soil type, temperature and depth below soil surface (Figs. 4–6).

The low sensitivity of $\phi_{\text{gas_min}}$ to soil organic matter content e_{org} likely has to do with the reduced microbial activity under the wet conditions at which oxygen stress occurs (through the moisture reduction factor for microbial respiration f_{ϕ} , Appendix A.5). This will have led to a relatively low microbial contribution to total oxygen consumption. The high sensitivity to temperature T is caused by the strong increase in respiration rate with T (Eqs. (1) and (10)). This sensitivity apparently dominated the sensitivity of diffusivities to T (Eqs. 5, 7, and 13) as the reverse should have led to decreased $\phi_{\text{gas_min}}$ with increased T . The sensitivity to soil depth z is due to depth dependent macro-scale diffusion distances.

All in all, the use of constant critical measures for oxygen stress should be avoided. $\phi_{\text{gas_min}} = 0.10$ is generally (e.g. Engelaar and Yoneyama, 2000; Leao et al., 2006;

Lipiec and Hatano, 2003; Zou et al., 2001) used as a critical value for aeration. However, Wesseling and van Wijk (1957) who introduced this threshold, already warned that $\phi_{\text{gas_min}} = 0.10$ ‘‘must be considered as preliminary’’. Despite this remark, this threshold is still applied in many studies.

Our simulations illustrate that in general, $\phi_{\text{gas_min}} = 0.10$ is too high for the abiotic conditions and plant characteristics considered in our research, except for those at higher temperatures and sandy soils. The real overestimation is even stronger, because Wesseling and van Wijk (1957) applied $\phi_{\text{gas_min}} = 0.10$ to the bottom end of the root zone, where $\phi_{\text{gas_min}}$ is higher than in the upper part of the root zone.

Our simulations were done for a temperate terrestrial grassland, but also characteristics of other crops or vegetation types can be used. $\phi_{\text{gas_min}}$ appeared to be sensitive to some of the plant characteristics, in particular to the respiration maintenance coefficient (k_m). This illustrates the importance of an accurate description of plant characteristics for the calculation of $\phi_{\text{gas_min}}$. Consequently, $\phi_{\text{gas_min}}$ will be different for other crops and vegetation types.

Fortunately, in many applications exact knowledge on actual plant characteristics is less important. Models like SWAP (Kroes et al., 2008) can be used with plant characteristics of a reference vegetation, instead of the actual vegetation, to assess a potential stress at a site. Such a measure, reflecting the oxygen status of the soil, can be used to predict the suitability of a site for certain natural vegetation types (e.g. Runhaar et al., 1997).

Improving oxygen stress thresholds

We used our model to simulate the reduction of water uptake by plant roots and herewith the sink term F that is involved in hydrological models like SWAP (Kroes et al., 2008) and HYDRUS (Šimůnek et al., 2005). Oxygen stress was coupled to F under the assumptions that: (i) root water uptake reaches a maximum ($F = 1$) upon obtaining the maximum growth respiration, (ii) root water uptake reaches zero ($F = 0$) when only maintenance respiration is feasible, and (iii) in between these thresholds, reduced root water uptake is directly proportional to reduced growth respiration. A maximum value of $\eta = 5$ was used to calculate the maximum growth respiration (Penning de Vries et al., 1979). This should be considered as an empirical value that seems valid in most cases, but deviations are likely to occur (Amthor, 2000). Although potential growth respiration and only maintenance respiration most likely correspond to $F = 1$ and $F = 0$, respectively, further research on the relationship between reduced respiration and reduced root water uptake in between these thresholds is recommended.

Although the linear shape of the Feddes-function seems valid (Fig. 5), constant threshold values for the points I and II (Fig. 1) are inappropriate for an accurate determination of oxygen stress. Reduction of root water uptake already starts at much drier conditions than according to the Feddes-function and additionally depends strongly on soil type and temperature. For instance, according to our model, oxygen stress on sandy loam (soil 5) occurs at a ca. 40 cm lower groundwater level than according to the Feddes-function (assuming hydrostatic equilibrium) (Fig. 5). For sites where the occurrence of oxygen stress could be an issue, i.e. at shallow groundwater levels, such a difference is considerable and cannot be ignored.

Assuming a linear relationship in between the two thresholds I and II (Fig. 1), our model can be used to generate reproduction functions to assess F for a variety of biotic and abiotic conditions (Appendix B). The advantage of such functions is that they speed-up the simulations considerably.

Applicability of the oxygen stress model

Our oxygen stress model can be applied to improve the simulation of both root water uptake and root growth in models that consider the soil-plant-atmosphere-continuum, like SWAP (Kroes et al., 2008). In this paper, we used it to substitute the sink term variable F at the wet side of the Feddes-function. However, other models for root water uptake can be improved with our approach as well. In several models (e.g. Doussan et al., 1998; Molz, 1981; Roose and Fowler, 2004), root water uptake is calculated on the basis of water absorption driven by hydraulic pressure differences between the root rhizosphere and the root xylem (passive transport). These types of models probably work well under conditions with sufficient oxygen supply to plant roots, but not in wetter conditions where water transport to roots is increasingly limited by metabolic processes (active transport) (see Section ‘‘The relation between oxygen stress and water uptake’’). Our model might be used to improve the pressure driven root water uptake models, by incorpo-

rating a root sink term F to adjust the water flux from the rhizosphere to the root xylem.

The simulation of root growth (e.g. WOFOST and SU-CROS (Van den Berg et al., 2002)), which is based on the net production of root biomass, can also be improved with the aid of our model. The production of root biomass is determined both by photosynthesis and by respiration (Cannell and Thornley, 2000). Our model might contribute to a better description of both processes: Carbon dioxide diffusion from the atmosphere into the plant is only possible when stomata are open. Consequently, photosynthesis is affected by root oxygen stress (Van Bodegom et al., 2008). Therefore, many crop growth models calculate the actual photosynthesis by linking it to potential photosynthesis and the relative transpiration rate (ratio of actual and potential transpiration = F) (Van den Berg et al., 2002). An accurate description of the relative transpiration and thus root water uptake is desired. Part of the carbohydrates produced by photosynthesis is used for respiration. Our model calculates the reduction in respiration rate of the roots due to oxygen stress, as a function of the actual (a)biotic conditions.

Our model is freely available from the internet in SWAP (Kroes et al., 2008). By including our model within SWAP, it has been integrated in a full hydrological modeling environment. Processes that are not directly involved in our model, but that might affect oxygen availability, like swelling and shrinking of soils and macro-pore flow, are accounted for in SWAP. Furthermore, with SWAP, relevant processes like heat flow and plant growth can be simulated.

Conclusions

In this paper, we showed that substantial differences in the minimum gas filled porosity of the soil – $\phi_{\text{gas_min}}$ – are especially related to soil type, soil temperature and soil depth. Consequently, constant values for $\phi_{\text{gas_min}}$ should be avoided, since they may result in large prediction errors of both transpiration and plant growth. The same holds, of course, for the fixed anaerobiosis pressure heads of the frequently used Feddes-function. To determine the oxygen stress experienced by roots accurately, we advocate an approach that takes account of relevant abiotic and biotic factors in an integrative manner.

Acknowledgements

This study was carried out in the framework of both Project A1 ‘Biodiversity in a changing environment: predicting spatio-temporal dynamics of vegetation’ of the Dutch National Research Program Climate Change and Spatial planning (www.klimaatvoorruimte.nl) and the joint research program of the Dutch Water Utility sector. We thank the editor and three anonymous reviewers for their valuable comments on the manuscript.

Appendix A. Calculation of model parameters

This appendix presents and justifies a number of equations that are part of our oxygen stress model.

Table B.1 Soil types from the Staring-series (Wösten et al., 2001)

Top soils	Description	Sub soils	Description
B1	Not loamy, very fine to moderately fine sand	O1	Not loamy, very fine to moderately fine sand
B2	Moderately loamy, very fine to moderately fine sand	O2	Moderately loamy, very fine to moderately fine sand
B3	Loamy, very fine to moderately fine sand	O3	Loamy, very fine to moderately fine sand
B4	Highly loamy, very fine to moderately fine sand	O4	Highly loamy, very fine to moderately fine sand
B5	Coarse sand	O5	Coarse sand
B6	Boulder clay	O6	Boulder clay
B7	Light sandy clay	O7	Brook loam
B8	Moderately sandy clay	O8	Light sandy clay
B9	Heavy sandy clay	O9	Moderately sandy clay
B10	Light clay	O10	Heavy sandy clay
B11	Moderately clay	O11	Light clay
B12	Heavy clay	O12	Moderately clay
B13	Sandy loam	O13	Heavy clay
B14	Silty loam	O14	Sandy loam
B15	Peaty sand	O15	Silty loam
B16	Sandy peat and peat	O16	Oligotrophic peat
B17	Peaty clay	O17	Mesotrophic and eutrophic peat
B18	Clayey peat	O18	Organic sublayer

Both top soils (B) and sub soils (O) are distinguished.

A.1. Root radius

The root radius a (m) of a cylindrical root was calculated following the method of De Willigen and Van Noordwijk (1987):

$$a = \sqrt{\frac{w}{\pi \cdot Y \cdot (1 - \phi_{\text{root}}) \cdot S} - \text{var}(a)}$$

with w the specific root mass (kg root m^{-1} root), Y the dry matter content of roots (–), ϕ_{root} the air filled root porosity (–), S the specific weight of non-airfilled root tissue (kg root m^{-3} root) and $\text{var}(a)$ the variance of a (m^2).

A.2. Organic carbon content

The organic carbon content of the soil μ (kg C m^{-3} soil) was calculated from the organic matter content of the soil ε_{org} (%) and the soil density ρ_{soil} (kg soil m^{-3} soil). This calculation is based on the assumption that soil organic matter weight consists of 48% of organic carbon.

$$\mu = 0.48 \cdot (\varepsilon_{\text{org}}/100) \cdot \rho_{\text{soil}}$$

A.3. Minimum oxygen concentration at the interface of the water-film and the soil air

The minimum oxygen concentration at the interface of the water-film and soil air, $C_{\text{min_int}}$ ($\text{kg O}_2 \text{ m}^{-3}$ root), was calculated following the method proposed by De Willigen and Van Noordwijk (1984). Their method is an extension of the method by Lemon and Wiegand (1962), describing the oxygen diffusion pathway from the gas phase of the soil to the root tissue, but additionally involves microbial respiration in the root rhizosphere, i.e. in the water-film that surrounds the root:

$$C_{\text{min}} = \frac{r_{\text{root_tot}} + r_{\text{waterfilm}}}{2 \cdot \pi \cdot D_{\text{root}}} \cdot \left\{ \frac{1}{2} + \frac{(\lambda - 1) \cdot \delta}{2} + \lambda \cdot \ln(1 + \Delta/a) - \frac{\lambda \cdot \delta \cdot (1 + \Delta/a)^2 \cdot \ln(1 + \Delta/a)}{(\Delta/a) \cdot (2 + \Delta/a)} \right\}$$

with

$$\lambda = D_{\text{root}}/D_{\text{waterfilm}}$$

$$\delta = r_{\text{waterfilm}}/(r_{\text{waterfilm}} + r_{\text{root_tot}})$$

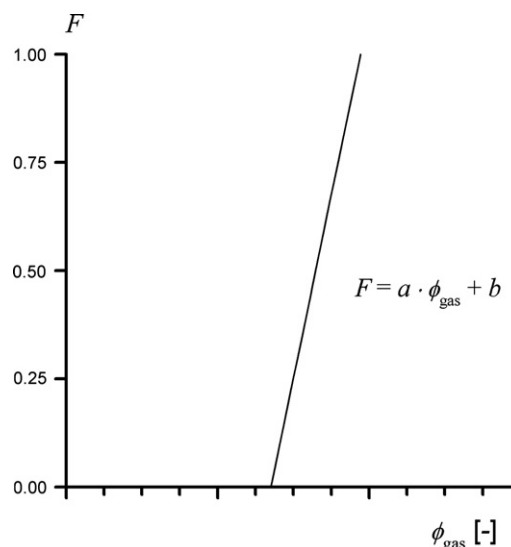


Figure B.1 Example of a repro-function to describe the relationship between ϕ_{gas} and F . Both the slope a and intercept b are functions soil type (Table B.1), soil temperature T_{soil} (K) and soil depth z (m) (Tables B.2 and B.3; Fig. B.2).

The oxygen consuming processes that are involved in the method of De Willigen and Van Noordwijk (1984) are both root respiration $r_{\text{root_tot}}$ ($\text{kg O}_2 \text{m}^{-1} \text{root d}^{-1}$) and respiration in the water-film $r_{\text{waterfilm}}$ ($\text{kg O}_2 \text{m}^{-1} \text{root d}^{-1}$). Since oxygen diffusion occurs through both the water-film and the root tissue, the diffusivities of oxygen through both media are included (D_{root} and $D_{\text{waterfilm}}$). The distance over which diffusion takes place is determined by the thickness of the water-film Δ and the root radius a .

A.4. Water-film thickness

The water-film thickness Δ (m) was approximated according to the procedure proposed by Simojoki (2000), which is based on soil water retention data. Δ was approximated by the difference between the calculated distance between

the pore centers (Barley, 1970 vide Simojoki, 2000) and the radii of the cylindrical gas filled pores (Simojoki, 2000):

$$\Delta = 2 \cdot \left(\sqrt{\frac{1}{\pi \cdot n(\varphi)} - \frac{2 \cdot \sigma}{\varphi}} \right)$$

with φ the matric potential of the soil moisture (Pa) and σ the surface tension of water (Nm^{-1}), that is given by the Eötvös rule: $\sigma = 0.07275 \cdot (1 - 0.002 \cdot (T_{\text{soil}} - 291))$. n is the length density of air filled pores (i.e. the number of air filled pores per unit area):

$$n(\varphi) = \int_0^\varphi \frac{-d\theta/d\varphi}{\pi \cdot 4 \cdot \sigma^2 / \varphi^2} d\varphi$$

which includes the derivative of the moisture retention curve according to Van Genuchten (1980):

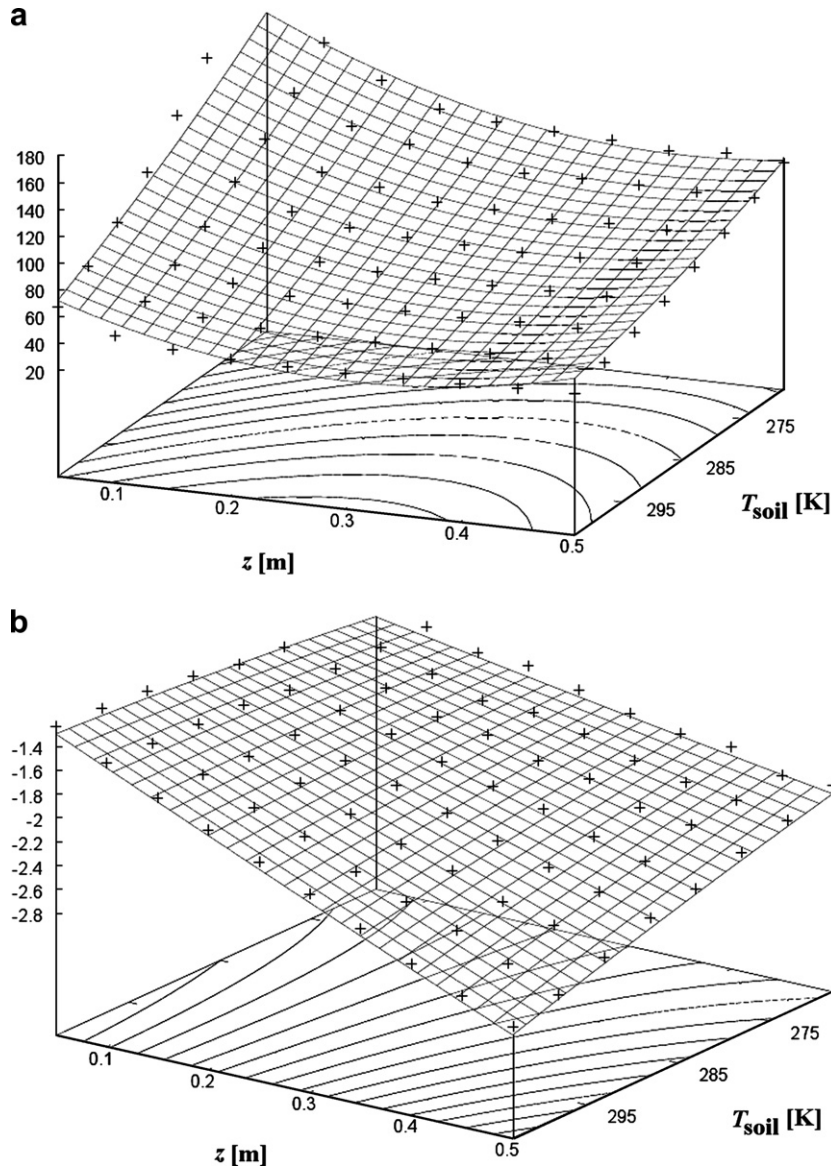


Figure B.2 Continuous functions, fitted on simulated data (crosses), of both the slope a (top figure) and intercept b of the re-profunction $F(\phi_{\text{gas}})$ (Fig. B.1) for soil type B8 (Table B.1).

$$\theta(\varphi) = \theta_{res} + \frac{\theta_{sat} - \theta_{res}}{(1 + (\alpha \cdot \varphi)^N)^M}$$

$$\frac{d\theta}{d\varphi} = \frac{(\theta_{sat} - \theta_{res}) \cdot \alpha \cdot (\alpha \cdot \varphi)^{N-1} \cdot (1 + (\alpha \cdot \varphi)^N)^{M-1} \cdot M \cdot N}{(((\alpha \cdot \varphi)^N + 1)^M)^2}$$

with θ_{sat} the saturated water content (–), θ_{res} the residual water content (–) and α (Pa⁻¹), M (–) and N (–) the Van Genuchten parameters.

A.5. Reduction of microbial respiration due to soil moisture availability

The factor f_φ that represents the reduction of microbial activity due to soil moisture availability is calculated according to Arora (2003) and Probert et al. (1998) fide Paul (2001). f_φ varies between 0.0 and 1.0, which represent max-

imum and minimum reduction, respectively. Arora (2003) proposed a reduction function for f_φ , in which f_φ is assumed to decrease linearly with the logarithm of matric potential ϕ between thresholds: φ_1 (25,000 Pa), φ_2 (762,500 Pa) and φ_3 (1,500,000 Pa). These thresholds are derived from Probert et al. (1998) fide Paul (2001) and incorporated in the formulation of Arora (2003):

$$f_\varphi = \begin{cases} 0.5 & \varphi < \varphi_{sat} \\ 1.0 - 0.5 \cdot \frac{\log(\varphi_1) - \log(\varphi)}{\log(\varphi_1) - \log(\varphi_{sat})} & \varphi_{sat} \leq \varphi < \varphi_1 \\ 1.0 & \varphi_1 \leq \varphi < \varphi_2 \\ 1.0 - \frac{\log(\varphi) - \log(\varphi_2)}{\log(\varphi_3) - \log(\varphi_2)} & \varphi_2 \leq \varphi < \varphi_3 \\ 0.0 & \varphi > \varphi_3 \end{cases}$$

with ϕ_{sat} the saturated matric potential (Pa). On the basis of field data, Cosby et al. (1984) proposed the following equation for ϕ_{sat} : $\phi_{sat} = 10^{(-0.0131 \cdot \epsilon_{sand} + 1.88)} \cdot 100$, with ϵ_{sand} the sand content of the soil (%).

Table B.2 Fitted parameters for the calculation of slope a in the repro-function $F = a \cdot \phi_{gas} + b$ ($0 \leq F \leq 1$): $a = a_1 T_{soil}^2 + a_2 z^2 + a_3 T_{soil} + a_4 z + a_5 T_{soil} z + a_6$

Soil type (Table B.1)	a_1	a_2	a_3	a_4	a_5	a_6	Residual standard error for a
B1	5.07e-03	2.40e+02	-4.39e+00	-6.31e+02	1.67e+00	9.08e+02	3.081
B2	1.20e-02	3.26e+02	-8.91e+00	-9.29e+02	2.49e+00	1.64e+03	4.791
B3	1.21e-02	3.64e+02	-9.09e+00	-9.90e+02	2.60e+00	1.70e+03	4.777
B4	1.67e-02	4.42e+02	-1.21e+01	-1.26e+03	3.34e+00	2.20e+03	6.448
B5	4.17e-03	1.93e+02	-3.72e+00	-5.28e+02	1.44e+00	7.77e+02	2.366
B6	2.11e-02	5.02e+02	-1.51e+01	-1.40e+03	3.69e+00	2.71e+03	7.223
B7	2.86e-02	5.57e+02	-1.97e+01	-1.67e+03	4.50e+00	3.41e+03	9.240
B8	1.75e-02	5.55e+02	-1.32e+01	-1.34e+03	3.31e+00	2.48e+03	7.140
B9	2.34e-02	6.00e+02	-1.70e+01	-1.40e+03	3.42e+00	3.09e+03	7.165
B10	3.12e-02	6.62e+02	-2.20e+01	-1.53e+03	3.65e+00	3.91e+03	7.722
B11	2.58e-02	6.42e+02	-1.83e+01	-1.61e+03	4.00e+00	3.26e+03	8.574
B12	2.50e-02	6.53e+02	-1.79e+01	-1.45e+03	3.40e+00	3.21e+03	8.596
B13	2.53e-02	5.97e+02	-1.79e+01	-1.72e+03	4.58e+00	3.18e+03	9.092
B14	2.82e-02	7.10e+02	-2.04e+01	-1.54e+03	3.56e+00	3.71e+03	8.186
B15	2.08e-02	4.72e+02	-1.46e+01	-1.37e+03	3.65e+00	2.57e+03	7.081
B16	1.99e-02	4.80e+02	-1.39e+01	-1.34e+03	3.47e+00	2.45e+03	6.845
B17	2.27e-02	6.31e+02	-1.62e+01	-1.58e+03	3.91e+00	2.91e+03	8.817
B18	2.23e-02	6.50e+02	-1.60e+01	-1.74e+03	4.45e+00	2.89e+03	10.200
O1	7.21e-04	1.76e+02	-1.59e+00	-4.33e+02	1.16e+00	4.52e+02	1.939
O2	3.75e-03	2.25e+02	-3.61e+00	-5.96e+02	1.59e+00	7.91e+02	2.803
O3	7.06e-03	2.86e+02	-5.91e+00	-7.52e+02	2.00e+00	1.19e+03	3.658
O4	1.29e-02	3.74e+02	-9.74e+00	-1.03e+03	2.72e+00	1.82e+03	5.126
O5	2.92e-03	1.86e+02	-3.06e+00	-5.07e+02	1.39e+00	6.85e+02	2.255
O6	3.00e-02	5.41e+02	-2.06e+01	-1.69e+03	4.61e+00	3.55e+03	9.061
O7	2.76e-02	6.63e+02	-1.95e+01	-1.67e+03	4.15e+00	3.48e+03	8.568
O8	1.85e-02	4.88e+02	-1.34e+01	-1.34e+03	3.50e+00	2.43e+03	7.169
O9	2.08e-02	5.46e+02	-1.50e+01	-1.50e+03	3.92e+00	2.72e+03	7.778
O10	1.85e-02	5.94e+02	-1.39e+01	-1.45e+03	3.60e+00	2.60e+03	7.867
O11	2.29e-02	6.33e+02	-1.67e+01	-1.65e+03	4.21e+00	3.05e+03	9.321
O12	2.60e-02	5.89e+02	-1.83e+01	-1.33e+03	3.12e+00	3.26e+03	6.613
O13	3.36e-02	6.27e+02	-2.29e+01	-1.40e+03	3.26e+00	3.95e+03	6.937
O14	3.84e-02	6.74e+02	-2.71e+01	-1.40e+03	3.21e+00	4.83e+03	7.449
O15	2.25e-02	6.16e+02	-1.66e+01	-1.37e+03	3.22e+00	3.05e+03	7.788
O16	1.88e-02	4.75e+02	-1.32e+01	-1.29e+03	3.31e+00	2.33e+03	6.737
O17	2.19e-02	5.40e+02	-1.53e+01	-1.50e+03	3.87e+00	2.70e+03	7.716
O18	1.98e-02	5.00e+02	-1.41e+01	-1.40e+03	3.67e+00	2.52e+03	7.372

A.6. Oxygen concentration in the atmosphere

The oxygen concentration in the atmosphere C_{atm} ($\text{kg O}_2 \text{ m}^{-3} \text{ air}$) was calculated according to the general gas law, assuming 21% oxygen in the atmosphere:

$$C_{\text{atm}} = 0.21 \cdot M_{\text{O}_2} \cdot \frac{p}{R \cdot T_{\text{air}}}$$

with M_{O_2} the molar mass of oxygen (kg mol^{-1}), p the atmospheric pressure (Pa), R the universal gas constant ($\text{m}^3 \text{ Pa K}^{-1} \text{ mol}^{-1}$) and T_{air} the air temperature (K).

A.7. Oxygen concentration in the gas phase of the soil

The oxygen concentration C ($\text{kg O}_2 \text{ m}^{-3} \text{ soil air}$) in the gas phase of the soil at soil depth z (m) (Fig. 2C) was calculated according to Cook (1995). His model is based on one-dimen-

sional oxygen diffusion in the soil. The diffusivity of the soil is given by D_{soil} ($\text{m}^2 \text{ d}^{-1}$). Additionally, his model involves a sink term that decreases exponentially with soil depth z .

Contrary to Cook (1995), we considered two separate sink terms in which both microbial and root respiration are involved (Fig. 2D). Each term is described both by a reference value at $z = 0$ ($R_{\text{microbial}_z0}$ in Eq. (12) and $R_{\text{root_tot}_z0}$ in Eq. (10) ($\text{kg O}_2 \text{ m}^{-3} \text{ soil d}^{-1}$)) and by a shape factor for the exponential decrease ($Z_{\text{microbial}}$ and Z_{root} (m) in Eqs. (11) and (9), respectively).

At $z = 0$, C equals the oxygen concentration in the atmosphere C_{atm} ($\text{kg O}_2 \text{ m}^{-3} \text{ air}$). Two different solutions for the oxygen concentration profile can be distinguished:

First, as for $z \rightarrow \infty$, $C \rightarrow$ constant and non-zero value. This occurs when:

$$Z_{\text{microbial}}^2 \cdot \frac{R_{\text{microbial}_z0}}{D_{\text{soil}}} + Z_{\text{root}}^2 \cdot \frac{R_{\text{root_tot}_z0}}{D_{\text{soil}}} < C_{\text{atm}}$$

Table B.3 Fitted parameters for the calculation of intercept b in the repro-function $F = a \cdot \phi_{\text{gas}} + b$ ($0 \leq F \leq 1$):
 $b = b_1 T_{\text{soil}}^2 + b_2 Z^2 + b_3 T_{\text{soil}} + b_4 Z + b_5 T_{\text{soil}} Z + b_6$

Soil type (Table B.1)	b_1	b_2	b_3	b_4	b_5	b_6	Residual standard error for b
B1	1.89e-04	-3.91e-01	-8.65e-02	2.11e+01	-8.61e-02	7.12e+00	0.027
B2	5.02e-05	-7.56e-02	-1.01e-02	1.80e+01	-7.27e-02	-2.81e+00	0.021
B3	5.36e-06	3.54e-01	1.20e-02	1.73e+01	-7.09e-02	-5.51e+00	0.026
B4	-2.67e-05	4.87e-02	3.03e-02	1.76e+01	-7.02e-02	-7.90e+00	0.022
B5	2.60e-04	-1.74e+00	-1.16e-01	2.28e+01	-8.99e-02	9.67e+00	0.039
B6	-1.23e-04	-6.11e-02	8.42e-02	1.66e+01	-6.63e-02	-1.51e+01	0.023
B7	-1.02e-04	8.54e-03	7.12e-02	1.76e+01	-7.06e-02	-1.33e+01	0.025
B8	-8.09e-05	2.23e-01	5.65e-02	1.62e+01	-6.61e-02	-1.08e+01	0.024
B9	-9.68e-05	1.56e-01	6.56e-02	1.67e+01	-6.76e-02	-1.21e+01	0.025
B10	-1.37e-04	-4.78e-02	8.94e-02	1.81e+01	-7.09e-02	-1.55e+01	0.028
B11	-1.71e-04	-2.25e-01	1.08e-01	1.68e+01	-6.46e-02	-1.78e+01	0.031
B12	-1.36e-04	-5.72e-01	8.92e-02	1.02e+01	-3.91e-02	-1.54e+01	0.040
B13	-1.19e-04	-8.68e-03	8.28e-02	1.77e+01	-6.97e-02	-1.54e+01	0.029
B14	-9.91e-05	-9.32e-01	7.13e-02	1.35e+01	-5.10e-02	-1.35e+01	0.053
B15	-7.90e-05	2.75e-02	5.85e-02	1.55e+01	-6.20e-02	-1.16e+01	0.016
B16	-7.91e-05	2.32e-01	5.71e-02	1.10e+01	-4.40e-02	-1.12e+01	0.017
B17	-2.21e-04	-5.23e-01	1.39e-01	1.44e+01	-5.42e-02	-2.27e+01	0.028
B18	-1.16e-04	-3.60e-01	7.85e-02	1.05e+01	-3.96e-02	-1.41e+01	0.029
O1	4.17e-04	-1.41e+00	-2.06e-01	2.42e+01	-9.84e-02	2.20e+01	0.043
O2	2.56e-04	-4.40e-01	-1.22e-01	2.19e+01	-8.92e-02	1.16e+01	0.029
O3	1.93e-04	-2.84e-01	-8.88e-02	1.96e+01	-8.08e-02	7.68e+00	0.032
O4	5.69e-05	-7.44e-02	-1.48e-02	1.80e+01	-7.36e-02	-2.01e+00	0.029
O5	5.21e-04	-1.81e+00	-2.61e-01	1.96e+01	-7.85e-02	3.01e+01	0.045
O6	-1.10e-04	6.88e-02	7.90e-02	1.77e+01	-7.11e-02	-1.48e+01	0.023
O7	-1.76e-04	-3.81e-01	1.11e-01	1.79e+01	-6.90e-02	-1.85e+01	0.031
O8	-2.38e-05	5.72e-01	2.47e-02	1.64e+01	-6.82e-02	-6.50e+00	0.026
O9	-4.68e-05	4.19e-01	3.84e-02	1.74e+01	-7.16e-02	-8.59e+00	0.028
O10	-1.10e-04	1.03e-01	7.32e-02	1.69e+01	-6.77e-02	-1.32e+01	0.027
O11	-1.48e-04	-3.36e-01	9.58e-02	1.78e+01	-6.94e-02	-1.64e+01	0.031
O12	-1.58e-04	1.36e-01	9.92e-02	1.56e+01	-6.18e-02	-1.65e+01	0.027
O13	-2.69e-04	-6.12e-01	1.66e-01	1.27e+01	-4.80e-02	-2.65e+01	0.042
O14	-6.34e-05	-4.27e-01	5.05e-02	1.73e+01	-6.82e-02	-1.06e+01	0.063
O15	3.08e-05	5.25e-02	-6.04e-03	8.44e+00	-3.54e-02	-2.00e+00	0.043
O16	-6.20e-05	3.40e-01	4.76e-02	9.54e+00	-3.85e-02	-9.98e+00	0.020
O17	-2.90e-05	3.99e-01	2.75e-02	8.07e+00	-3.30e-02	-6.73e+00	0.020
O18	-6.76e-05	4.41e-01	5.01e-02	1.50e+01	-6.10e-02	-1.01e+01	0.023

then

$$C = C_{\text{atm}} - \left(z_{\text{microbial}}^2 \cdot \frac{R_{\text{microbial}_z0}}{D_{\text{soil}}} \right) \cdot \left(1 - \exp\left(-\frac{z}{z_{\text{microbial}}}\right) \right) - \left(z_{\text{root}}^2 \cdot \frac{R_{\text{root_tot}_z0}}{D_{\text{soil}}} \right) \cdot \left(1 - \exp\left(-\frac{z}{z_{\text{root}}}\right) \right)$$

Second, as for $z \rightarrow \infty$, $C \rightarrow 0$. This occurs when:

$$z_{\text{microbial}}^2 \cdot \frac{R_{\text{microbial}_z0}}{D_{\text{soil}}} + z_{\text{root}}^2 \cdot \frac{R_{\text{root_tot}_z0}}{D_{\text{soil}}} \geq C_{\text{atm}}$$

then

$$C = C_{\text{atm}} - \left(z_{\text{microbial}}^2 \cdot \frac{R_{\text{microbial}_z0}}{D_{\text{soil}}} \right) \cdot \left(1 - \frac{z}{z_{\text{microbial}}} \cdot \exp\left(-\frac{L}{z_{\text{microbial}}}\right) - \exp\left(-\frac{z}{z_{\text{microbial}}}\right) \right) - \left(z_{\text{root}}^2 \cdot \frac{R_{\text{root_tot}_z0}}{D_{\text{soil}}} \right) \cdot \left(1 - \frac{z}{z_{\text{root}}} \cdot \exp\left(-\frac{L}{z_{\text{root}}}\right) - \exp\left(-\frac{z}{z_{\text{root}}}\right) \right)$$

where z at which $C = 0$, given by L (m) (Fig. 2C) can be found iteratively through the Newton–Raphson method:

$$f_i = 0 = C(L)$$

$$f'_i = -\frac{R_{\text{microbial}_z0}}{D_{\text{soil}}} \cdot L \cdot \exp\left(-\frac{L}{z_{\text{microbial}}}\right) - \frac{R_{\text{root_tot}_z0}}{D_{\text{soil}}} \cdot L \cdot \exp\left(-\frac{L}{z_{\text{root}}}\right)$$

$$L_{i+1} = L_i - \frac{f_i}{f'_i}$$

Appendix B. Repro-functions for the reduction of root water uptake of a temperate grassland under oxygen stress

We used simulations with our process-based model for oxygen stress to describe root water uptake reduction F as a continuous function of gas-filled porosity ϕ_{gas} , soil temperature T_{soil} and soil depth z . These repro-functions are based on the following assumptions and restrictions:

- The repro-functions are only valid for the plant characteristics of temperate terrestrial natural grasslands (Table 2) and for soil types that resemble the Staring series of Wösten et al. (2001) (Table B.1).

- Between minimum and maximum oxygen deficiency (points I and II in Fig. 1), a linear relationship between F and ϕ_{gas} is assumed (Fig. B.1).

- The air temperature T_{air} equals T_{soil} (K).

- The organic matter content $\varepsilon_{\text{org}} = 10\%$ for all soils (our model, see section ‘‘Sensitivity of $\phi_{\text{gas_min}}$ and F to environmental parameters’’ appeared to be hardly sensitive to ε_{org}).

- The repro-functions were derived for limited ranges of abiotic conditions: $265 \text{ K} \leq T_{\text{soil}} \leq 303 \text{ K}$ and $0.05 \leq z \leq 0.5 \text{ m}$.

Assuming linearity, the general shape of the relationship between F and ϕ_{gas} , can be described as $F = a \cdot \phi_{\text{gas}} + b$ ($0 \leq F \leq 1$; Fig. B.1), where both a and b were approximated as functions of T_{soil} and z (Fig. B.2):

$$a = a_1 T_{\text{soil}}^2 + a_2 z^2 + a_3 T_{\text{soil}} + a_4 z + a_5 T_{\text{soil}} z + a_6$$

$$b = b_1 T_{\text{soil}}^2 + b_2 z^2 + b_3 T_{\text{soil}} + b_4 z + b_5 T_{\text{soil}} z + b_6$$

We derived parameter values a_{1-6} and b_{1-6} for different soil types through curve fitting on simulated data in the following way. First, we simulated F as function of ϕ_{gas} and we computed the slope a and intercept b by linear regression. This was done for different soil types (Table B.1), 8 values for T_{soil} ($268 \text{ K} \leq T_{\text{soil}} \leq 303 \text{ K}$ and a step size of 5 K) and 10 values for z ($0.05 \leq z \leq 0.5 \text{ m}$ and a step size of 0.05 m). Second, for each soil type we derived values of a_{1-6} and b_{1-6} by non-linear least square fitting in R (www.r-project.org) on all 80 points $a(T_{\text{soil}}, z)$ and $b(T_{\text{soil}}, z)$ respectively. Examples of the thus obtained functions for a and b are presented in Fig. B.2. The results for the fitted parameter values for all soils, including the fit statistics, are presented in Tables B.2(a) and B.3(b).

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