Supplement of

Inorganic carbon fluxes across the vadose zone of planted and unplanted soil mesocosms

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Fig. S1. Time course of pCO$_2$, volumetric water content (VWC), temperature, alkalinity (Alk.), DIC and pH on measurement days throughout depth during barley growth (treatment #2) and after harvest. Measurements at 45 and 63 cm depth were excluded for clarification of the figure but followed the same trends as measurements at 13–56 cm. Note the different x axis scale for the subfigures.
Fig. S1 (continued). Time course of pCO$_2$, volumetric water content (VWC), temperature, alkalinity (Alk.), DIC and pH on measurement days throughout depth in unplanted soil. Measurements at 45 and 63 cm depth were excluded for clarification of the figure but followed the same trends as measurements at 13–56 cm.
Fig. S2: Log activities of $\text{Al}^{3+}$ vs. $H^+$ as compared to the equilibrium line for $\text{Al(OH)}_3(a)$ and log activities of $\text{CO}_3^{2-}$ vs. $\text{Ca}^{2+}$ as compared to the equilibrium line for $\text{CaCO}_3$ of pore water in A and C horizons on day 71 (series 2 mesocosms only). Samples were analyzed by ICP-MS (Elan6100DRC, Perkin Elmer, CAN), and concentrations were corrected for dilution by the acid added during a previous alkalinity titration. Saturation indices of different minerals in the mesocosms were calculated with PHREEQC software (Parkhurst and Appelo, 2011). Concentrations of the major anions $\text{NO}_3^-$ and $\text{SO}_4^{2-}$ were set to 62 and 96 mg L$^{-1}$, respectively, as given by the Hoagland solution composition (Hoagland and Amon, 1950). Solutions were charged balanced by adding either $\text{Li}^+$ or $\text{Cl}^-$ until electro neutrality.

The pore water was supersaturated for amorphous aluminum hydroxide, $\text{Al(OH)}_3(a)$, and this indicates the possible precipitation of a gibbsite-type mineral. The soil solutions were subsaturated for calcite, $\text{CaCO}_3$, indicating the possible dissolution of lime particles added to the field site. The relations between measurement points and the equilibrium lines were less parallel in the C horizon, indicating less control of either aluminum hydroxide or calcite in the subsoil. Activities of $H^+$ were generally lower in the pore water samples from planted soil than in unplanted soil, while activities of $\text{CO}_3^{2-}$ were slightly elevated.
Fig. S3: Simulated nutrient uptake rates of remaining nutrients.
Fig. S4: Simulated movement of chloride tracer applied at a concentration of $0.92 \times 10^{-5}$ moles L$^{-1}$. Combined action of evaporation and transpiration increased tracer concentration ~3 times. Evapotranspiration caused a peak in the tracer concentration in the C horizon. Evaporation causes steep increases in the tracer concentration at the very top of the mesocosm.
Fig. S5: Measured and modeled cumulative drainage and volumetric water content (VWC) in barley mesocosm 5.
**Text S1: Calculation of theoretical diffusion coefficients**

Theoretical bulk diffusion diffusivities, $D$, were calculated using the empirical formulas of Rogers and Nielson (1991) and Andersen (2000) (Eq. 1-3).

$$D = D_e \beta$$  \hspace{1cm} (1)

$$D_e = D_0 \varepsilon \exp(-6m\varepsilon - 6m^{14}\varepsilon)$$  \hspace{1cm} (2)

$$\beta = \varepsilon_a + L\varepsilon_w + K\rho_b$$  \hspace{1cm} (3)

Where $D_e$ is the effective diffusion coefficient ($m^2 s^{-1}$), $D_0$ is the diffusion coefficient in air ($m^2 s^{-1}$), $\varepsilon$ is the total porosity ($m^3 m^{-3}$), $\varepsilon_a$ is the air-filled porosity ($m^3 m^{-3}$), $\varepsilon_w$ is the water-filled porosity ($m^3 m^{-3}$), $m$ is the water saturation ($\varepsilon_w / \varepsilon$) ($m^3 m^{-3}$), $L$ is the Ostwald coefficient (equals approx. 0.36 at 10°C and 0.23 at 25°C (Clever, 1979)) and $K$ is the radon surface sorption coefficient ($kg m^{-3}$) (Rogers and Nielson, 1991), and $\rho_b$ is the soil bulk density ($kg m^{-3}$).

In the calculations $\varepsilon_w$ was set to 0.2 and 0.1 ($m^3 m^{-3}$) for the A and C horizon, respectively, $\rho_b$ was 1.45 and 1.53 $kg m^{-3}$ for the A and C horizon, respectively, and $K$ was assumed to be 0. $L$ was set to 0.26. Total porosities of the A and C horizon were 0.45 and 0.43, respectively.
Table S1: Parameters used in the modeling of soil CO₂ fluxes. DW= dry weight.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Value</th>
<th>Calculation/Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_{\text{init}} )</td>
<td>Initial root mass</td>
<td>2.0 g DW</td>
<td>Calculated from the measured root mass (Table 3) assuming linear root growth</td>
</tr>
<tr>
<td>( r )</td>
<td>Root growth rate</td>
<td>2.4 ( \times 10^{-6} ) g s⁻¹</td>
<td>Calculated from the measured root mass 65.5 days after germination (Table 3) and assuming linear root growth</td>
</tr>
<tr>
<td>( RMI )</td>
<td>Root mass index</td>
<td></td>
<td>Calculated by ( R_{\text{init}} + (r \times \text{time}) )</td>
</tr>
<tr>
<td>( \gamma_{s0} )</td>
<td>Optimum microbial respiration</td>
<td>0.8 µmol m⁻² s⁻¹ g⁻¹ DW⁻¹</td>
<td>Average “optimum” respiration in planted mesocosms divided by the root mass 65.5 days after germination (Table 3) and by a factor 2 for equal division between root and microbial respiration</td>
</tr>
<tr>
<td>( \gamma_{p0} )</td>
<td>Optimum root respiration</td>
<td>0.8 µmol m⁻² s⁻¹ g⁻¹ DW⁻¹</td>
<td></td>
</tr>
<tr>
<td>( a )</td>
<td>Scaling factor for depth dependency of microbial respiration</td>
<td>0.0015 m⁻¹</td>
<td></td>
</tr>
<tr>
<td>-</td>
<td>Boundary layer height</td>
<td>0.02 m</td>
<td></td>
</tr>
</tbody>
</table>
References


5 Nielsen, N. E.: Forløbet af rodudvikling, næringsstofoptagelse of stofproduktion hos byg, dyrket på frugtbar morænelerjord, Royal Veterenary and Agricultural University, Copenhagen, DK, 1982.


