Supplementary Information

Text S1

Detailed Information about the laboratory experiment

Soil preparation, P treatments, and pot filling

A pot trial was set up (2017) in a greenhouse located at the Sokoine University of Agriculture in Morogoro (6°50'53.9"S, 37°39'31.3"E; Tanzania). The averages of the daily minimum and maximum temperatures were respectively 21.9 °C and 33.4 °C. Initially, a P-deficient soil (0.035 mg P l^{-1} in soil solution, measured by ICP-MS after a water extraction) was collected from an upland rice field in Matombo (07°02'46.8"S; 37°47'11.6"E; Tanzania). This soil was classified as a ferralsol (*World Reference Base for Soil Resources*) and was characterized by a soil pH($CaCl_2$) = 5.7, a particle size distribution of 9% sand, 57% silt, 34% clay, and an oxalate extractable Al_{ox} = 1073 mg kg^{-1}, Fe_{ox} = 1730 mg kg^{-1}, Mn_{ox} = 2559 mg kg^{-1}, P_{ox} = 122 mg kg^{-1}. After sampling, the bulk soil was shade dried, crushed to an aggregate size of 4 mm, and amended with salts of NH_4NO_3, KCl, $CaCl_2$, $MgSO_4$, $ZnSO_4$, $CuSO_4$, H_3BO_3 and Na_2MoO_4 at rates of 37 mg N kg^{-1}, 95 mg K kg^{-1}, 16 mg Mg kg^{-1}, 21 mg S kg^{-1}, 3.5 mg Zn kg^{-1}, 0.04 mg B kg^{-1}, 0.08 mg Cu kg^{-1}, and 0.03 mg Mo kg^{-1} soil, in order to avoid any deficiency other than P.

As P generally accumulates in the topsoil, no P was initially added to the bulk soil in order to mimic a P deficient subsoil. Large pots (height: 55cm, diameter: 16cm) were then filled with 7.3 kg of the P deficient subsoil. The remaining of this bulk soil was then subjected to three different P treatments. One third was amended with a non-limiting amount of ground Triple Super Phosphate (TSP) (70.8 mg P $kg_{topsoil}^{-1}$ or 354 mg P per pot) up to a theoretical P concentration of 0.5 mg P l^{-1} in soil solution (PlusP), which was based on the previously determined P adsorption isoterm. Another third was amended with a sub-optimal amount of ground TSP (25.0 mg P $kg_{topsoil}^{-1}$ or 125.2 mg P per pot) up to a theoretic P concentration of 0.1 mg P l^{-1} in soil solution (SubP). The remaining part was not amended with TSP (NoP), and $CaCl_2$ was used to equalize the amended Ca in all treatments. Pots were then filled with 5 kg of topsoil, affixed on top of each

subsoil. The bulk density of the dry soil in the pot was 1.29 g cm^{-3}. The layer of the subsoil was 30 cm and the topsoil was 20 cm thick. Pots were then irrigated to bring the whole pot to field capacity (38% w/w).

Sowing, maintenance, and water treatments

One pre-germinated seed of the typical upland rice variety (NERICA4) was sown into the pots (1 cm depth) at the center of the surface, which closely relates to a conventional spacing density of 20x20 cm for rice on the field. NERICA4 is developed by the Africa Rice Center using interspecific crosses between *Oryza sativa* (Asian rice) and *Oryza glaberrima* (African rice). NERICA4 is an upland rice variety known for its drought tolerance but it is relatively susceptible to low P.

Two top dressings of NH_4NO_3 (in solution) were later applied at a rate of 349 mg N per pot at 21 and 34 days after sowing (DAS). An additional top dressing of $ZnSO_4$, $ZnCl_2$, KCl, and $MgSO_4$ were added to each pot at rates of 0.27 g Zn, 0.58 g K, 0.16 g S, and 0.11 g Mg.

Pots were daily irrigated to field capacity (based on pot weight) until 25 DAS, and two contrasting water treatments were then initiated and maintained until the end of the trial. Half of the pots were daily irrigated to field capacity (FC), while the other half was subjected to drying periods (DP). In order to represent drying cycles during erratic rainfall, pots were re-watered up to field capacity after a period of ca. six days (preset as an average period of drying). Each treatment combination was replicated four times. The amount of irrigated water was consistently monitored to assess evapotranspiration, water use, and water productivity. An estimate of the evaporation was monitored by daily weighing and re-irrigating six unsown pots, randomly placed through the experiment.

Text S2

Detailed information on the model descriptors and the mathematical equations

The nutrient transfer in the soil is described by the transport equation with consideration of nutrient sorption onto the soil matrix:

$$\frac{\partial(\theta c_l + \rho_b c_s)}{\partial t} - \nabla.\left(D_e \nabla c_l - \nabla.(c_l v)\right) - q_{\frac{croot}{soil}} = 0, \qquad \textit{Equation 1}$$

where

c_l – mass concentration in liquid phase [M L^{-3}]

θ – soil water content [-]

ρ_b – soil bulk density [M L^{-3}]

v – Darcy flow in soil [L T^{-1}]

D_e – effective diffusive coefficient, calculated according to Millington and Quirk (1961) [L^2 T^{-1}]

c_s – mass concentration in soil matrix [M M^{-1}], related to c_l by the Freundlich isotherm:

$$c_s = F_K c_l^n, \qquad \textit{Equation 2}$$

where n [-], F_K [M^{-n} L^{3n}] are the Freundlich coefficients.

$q_{\frac{croot}{soil}}$ – nutrient uptake by root from soil [M L^{-3} T^{-1}] which is described by Michaelis Menten kinetics

$$q_{\frac{croot}{soil}} = \frac{v_m c_{l\_int}}{K_m + c_{l\_int}} S_{root}, \qquad \textit{Equation 3}$$

where c_{l_int} - nutrient concentration at root surface [M L^{-3}], V_m - maximum uptake rate [M T^{-1} L^{-2}], K_m - Michaelis Menten constant [M L^{-3}] and S_{root} is root surface area per unit soil volume [L^2 L^{-3}].

The continuum multiscale coupling approach for growing root systems

In this study, the development of the root architecture (i.e. root growth starting from day 0) is first simulated according to the measured and estimated root parameters presented in Table 2, before coupling the root system with the computations of water flow and solute transport. In this way, simulated root characteristics fit well to the observed characteristics under the different scenarios and the age of each root segment is defined.

Hence, for the simulation of water flow and solute transport in the soil-root system during a certain time step, only root segments that are 'born' before that specific time step are included in the computation of the sink terms for water and nutrient uptake. In this way, we mimic root growth although we already know the final root architecture.

The rhizosphere scale models around different root segments which share a common soil control volume have a cylindrical domain R_i which is proportional to radius r_i of the root segment and depends on the total root surface in the soil volume V_s.

$$R_i = \sqrt{\frac{r_i^2 V_s}{\pi \sum r_j^2 l_j}}, \qquad \textit{Equation 4}$$

where $\pi \sum r_j^2 l_j$ is the total root surface of the already born segments, which increases over time due to the emergence of new root segments that grow into the soil control volume. As a result, the share of exploitable soil volume by each root segment and thus the radius R_i reduces during the simulation. This is implemented in the multiscale model by decreasing the outer radius of the existing cylindrical domains accordingly while keeping the already existing concentration profile near the existing root surfaces and creating new rhizosphere models for the newly born root segments.

We ensured the conservation of mass in the multiscale model which is described as follows:

To represent the changing rhizosphere models of the root segments, we discretized the cylindrical rhizosphere using 10 static elements and one dynamic element at the outer boundary which adapts its length due to the updated rhizosphere radius. The length of the static part is defined as 80% of the final rhizosphere domain radius (when the root system is at its final development stage and all root segments in the soil voxel have emerged). This static part therefore corresponds with the rhizosphere around a root segment that is not 'encroached' by new emerging root segments. The dynamic element has a varying outer vertex, which changes its position according to the updated radius. The value of 80% was chosen to avoid zero length of the dynamic element. In every time step, the boundary fluxes for the rhizosphere models are also updated with consideration of new rhizosphere models. The initial conditions in new rhizospheres are defined such that the total mass in a given soil control element is equal to the total mass in all the new rhizosphere and in the existing ones. When a new root enters a specific soil control volume, the outer radius of the soil cylinders around each root is computed according to Eqn. (4). The outer radius of the soil cylinder around the existing roots is reduced by clipping the domain from the outer end, keeping the already existing concentration profile near the root surface. For the soil cylinders around the new roots, we assume that the concentration is initially homogeneous and according to Eqn. 5, i.e. the distribution with distance from the root surface is assumed constant for the new roots. Indeed, the reality might be different, but it is not feasible to estimate the initial distribution for the new root as we do not resolve the position of each root segment inside the soil control volume.

The total nutrient concentration in the new rhizosphere c_{total} [M L^{-3}] is computed as:

$$c_{total} = \frac{c_{totalSoil} V_{soil} - \sum m_{rhizo}}{V_{soil} - \sum V_{rhizo}}, \qquad \textit{Equation 5}$$

where

$c_{totalSoil}$ - total nutrient concentration in the soil control volume [M L^{-3}]

V_{soil} - the soil control volume [L^3]

m_{rhizo} - the nutrient mass in the updated previously existing rhizosphere volumes [M]

V_{rhizo} - the updated previously existing rhizosphere volume after the growth of new root segments in the soil [L^3]

Since the coupled rhizosphere –macro scale model does not represent the actual spatial distribution of the cylindrical rhizosphere models around each root segment within a soil voxel, it is assumed that the initial concentration distribution in the cylinders around the newly emerging root segment is uniform. This is furthermore consistent with the assumed axisymmetric concentration distributions in the cylindrical rhizosphere models that consider neither concentration gradients in the axial direction nor in the direction perpendicular to the radial direction. It must be noted that the new rhizosphere models emerge in the region outside of the static regions around the already existing segments. Since the concentration gradients decrease strongly with distance from the already existing root surfaces, the concentration gradients in the zones where the new root segments emerge are small compared with the gradients that emerge from uptake by new segments.

Root system modelling with different lateral root types

Based on the experimental data, we reconstructed the rice root systems by using the root architecture model CRootBox (Schnepf et al. 2018). In this model, each single root follows negative exponential growth and is characterized by the following parameters: the maximum root length, the initial growth rate, the lengths of the basal and apical zones, the interbranch distance, the branching angle, as well as the tropism parameters. Originally, in CRootBox a constant time interval between the emergence of two consecutive nodal roots is used. In this study, in order to adapt to the experimental data, the emergence of the nodal roots is set to be more flexible by a negative exponential function,

$$n = N \frac{(1- e^{\frac{k}{N}t})}{(1- e^{\frac{k}{N}T})}, \qquad \textit{Equation 6}$$

where

n - the total number of nodal roots at time t [T]

N - the total number of nodal roots at the final time T [T]

k - the emerging coefficient which is estimated in calibration [T^{-1}]

It can be shown that $n=N\ (1-\ e^{\frac{k}{N}t})/(1-\ e^{\frac{k}{N}T})$,

Equation 6 becomes linear in time as k tends to zero, i.e., $\lim_{k\to 0} n = \frac{N}{T}t$.

The root system of rice was characterized as having several nodal roots and two types of lateral roots: the short and thin laterals (S-type) versus the longer ones (L-type). With a small radius and short length, the S-type roots emerge along the whole nodal root, but their presence is most abundant on the basal part of nodal roots and they mainly grow in the topsoil layer. On the other hand, the L-type roots are more abundant on the deeper layer of the nodal roots, and they mainly grow in the deeper soil layers with further 2nd order lateral branches which are here considered as part of the L-type lateral. To describe the gradual change of first order lateral formation along the nodal roots, a logistic probability function of lateral type was implemented to calibrate according to the observed root mass distribution:

$p = \frac{1}{1+ e^{-s(z-z_0)}}$, *Equation 7*

where

p - the probability of S-type lateral roots at depth z [L]

s - the transition steepness from S-type to L-type lateral root [L^{-1}]

z_0 - is the transition depth from S-type to L-type lateral root [L] (z

Similarly, it is also noticed that the branching distance of laterals varies along nodal roots. Therefore, a scaling factor function for the interbranch distance depending on the depth was implemented:

$$k_s = \frac{k_{s,\infty}-1}{1+e^{-s(z-z_0)}} + 1, \qquad \textit{Equation 8}$$

where k_s [-] is the scaling factor of the interbranch distance of first-order laterals (S and L) and at depth z. The scaling factor goes from 1 at z = -∞ to $k_{s,\infty}$ [-] at z=+∞. z_0 is the depth where $k_s=(1+k_{s,\infty})/2$.