**Image based modeling of nutrient movement in and around the rhizosphere**

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**Summary**

Using rigorous mathematical techniques and image based modelling we quantify the effect of root hairs on nutrient uptake. In addition we investigate how uptake is influenced by growing root hairs.

1. **Abstract**

In this paper we develop a spatially explicit model for nutrient uptake by root hairs based on X-ray Computed Tomography images of rhizosphere soil structure. This work extends our previous study ([Keyes et al., 2013](#_ENREF_17)) to larger domains and, hence, is valid for longer times. Unlike the model used in ([Keyes et al., 2013](#_ENREF_17)), which considered only a small region of soil about the root, we consider an effectively infinite volume of bulk soil about the rhizosphere. We ask the question “at what distance away from root surfaces do the specific structural features of root-hair and soil aggregate morphology not matter because average properties start dominating the nutrient transport?” The resulting model captures bulk and rhizosphere soil properties by considering representative volumes of soil far from the root and adjacent to the root respectively. By increasing the size of the volumes we consider, the diffusive impedance of the bulk soil and root uptake are seen to converge. We do this for two different values of water content which provides two different geometries. We find that the size of region for which the nutrient uptake properties converge to a fixed value is dependent on the water saturation. In the fully saturated case the region of soil which we need to consider is only of radius 1.1 mm for poorly soil-mobile species such as phosphate. However, in the case of a partially saturated medium (relative saturation 0.3) we find that a radius of 1.4 mm is necessary. This suggests that, in addition to the geometrical properties of the rhizosphere, there is an additional effect on soil moisture properties which extends further from the root and may relate to other chemical changes in the rhizosphere which are not explicitly included in our model.

**Keywords:**

Rhizosphere, X-ray CT, structural imaging, phosphate, plant-soil interaction

**Abbreviations:**

CT – Computer Tomography

**Short title for page headings:** Modelling nutrient uptake

**Introduction**

The uptake of phosphate and other low mobility nutrients is essential for plant growth and, hence, global food security ([Barber, 1984](#_ENREF_3); [Nye and Tinker, 1977](#_ENREF_23); [Tinker and Nye, 2000](#_ENREF_27)). However, the overuse of inorganic fertilizers has caused an accumulation of phosphate in European soils which potentially causes eutrophication ([Gahoonia and Nielsen, 2004](#_ENREF_8)). Hence, there is a need to optimize the efficiency of phosphate uptake not only to increase crop yields, but also to minimize the detrimental effects of excess phosphate on the environment.

Plants are known to uptake nutrients both through their roots and root hairs ([Datta et al., 2011](#_ENREF_6)). Root hairs are thought to play a significant role in the uptake of poorly soil-mobile nutrients such as phosphate, water uptake, plant stability and microbial interactions ([Datta et al., 2011](#_ENREF_6); [Gahoonia and Nielsen, 2004](#_ENREF_8)). In order to quantify the role of root hairs in the uptake of poorly soil-mobile nutrients, such as phosphate, a detailed understanding of the root-hair morphology and the region of soil around the root, known as the rhizosphere ([Hiltner, 1904](#_ENREF_14)), is required. This is because the properties of soil in the rhizosphere are thought to be significantly different due to soil microbial interactions and compaction of soil by the root ([Aravena et al., 2010](#_ENREF_1); [Aravena et al., 2014](#_ENREF_2); [Daly et al., 2015](#_ENREF_4); [Dexter, 1987](#_ENREF_7); [Whalley et al., 2005](#_ENREF_31)).

Early models for nutrient movement in soil treated the rhizosphere as a volume averaged continuum ([Barber, 1984](#_ENREF_3); [Ma et al., 2001](#_ENREF_21); [Nye and Tinker, 1977](#_ENREF_23)). More recently models for nutrient movement have been derived and parametrized for dual porosity soil ([Zygalakis et al., 2011](#_ENREF_33)) and for soil adjacent to cluster roots ([Zygalakis and Roose, 2012](#_ENREF_34)). These models were based around the technique of homogenization ([Hornung, 1997](#_ENREF_15); [Pavliotis and Stuart, 2008](#_ENREF_24)), a multi-scale technique which enables field scale equations to be derived and parametrized based on underlying continuum models.

To obtain a better understanding of processes occurring in the rhizosphere, in comparison to the surrounding bulk soil, non-invasive measurements of the plant root and soil structure are essential ([George et al., 2014](#_ENREF_9); [Hallett et al., 2013](#_ENREF_13)). Three dimensional imaging of plant roots in-situ using X-ray Computed Tomography (CT) is a rapidly growing field ([Aravena et al., 2010](#_ENREF_1); [Aravena et al., 2014](#_ENREF_2); [Hallett et al., 2013](#_ENREF_13); [Keyes et al., 2013](#_ENREF_17); [Tracy et al., 2010](#_ENREF_29)). Using these techniques sub-micron resolutions can be achieved enabling the root hair morphology to be visualized ([Keyes et al., 2013](#_ENREF_17)).

In addition to direct in-situ visualization of plant-soil interaction, the use of X-ray CT also provides the means to apply numerical models describing the diffusion of nutrients directly to the imaged geometries ([Aravena et al., 2010](#_ENREF_1); [Aravena et al., 2014](#_ENREF_2); [Daly et al., 2015](#_ENREF_4); [Keyes et al., 2013](#_ENREF_17); [Tracy et al., 2015](#_ENREF_28)). This approach has been used to quantify the effectiveness of root hairs in saturated soil conditions ([Keyes et al., 2013](#_ENREF_17)) using a diffusion model originally developed for mycorrihzal fungi ([Schnepf et al., 2011](#_ENREF_26)). However, the study in ([Keyes et al., 2013](#_ENREF_17)) considered a small volume of soil adjacent to the root. This volume extended *c.*  from the root surface and had a zero flux boundary condition on the outer surface. Hence, once the phosphate immediately adjacent to the root was depleted the uptake of nutrients into the root stopped. This, whilst accurate for the experimental situation considered, limited the time frame for which the model was applicable to *c.* 3 hours.

In this paper we extend the work of ([Keyes et al., 2013](#_ENREF_17)) to include both bulk and rhizosphere soil. The key aims of this study are to develop an image based modelling approach which is applicable to root hairs surrounded by a large/infinite bulk of soil, to understand how root hairs contribute to nutrient uptake at different soil water content and to estimate the effects of root hair growth on nutrient uptake. We have chosen to model a single root in a large/infinite volume of soil, rather than multiple roots competing for nutrients for a number of reasons. Firstly, we want to compare our model to established models for nutrient uptake which are applied in this geometry ([Roose et al., 2001](#_ENREF_25)). Secondly, whilst some models consider root-root competition, ([Barber, 1984](#_ENREF_3)), these models are applied in a cylindrical geometry. Hence, any competition is provided by a ring of roots at a distance from the root under consideration. In order to accurately capture roots at a given root density additional assumptions and approximations would be required. Finally, our aim is to study the role of root hairs on the uptake of a single root. Hence, we have chosen to study a geometry which captures and isolates this effect. The modelling strategy developed in this paper will provide a framework for future modelling studies to consider how different root hair morphologies influence uptake. In addition it will provide a new level of understanding in to the role or root hairs in nutrient uptake as the root system begins to develop.

The bulk soil properties are derived using multi-scale homogenization combined with image based modelling in a similar manner to ([Daly et al., 2015](#_ENREF_4)). The resulting equations are solved analytically and are patched to an explicit image based geometry for the rhizosphere using a time dependent boundary condition. Reducing the bulk soil to a single boundary condition allows us to capture the full geometry and topology of the plant-root-soil system without the need for excessive computational resources and has particular relevance to poorly soil-mobile species such as phosphate, potassium and zinc. The model describes phosphate uptake by roots and root hairs in an effectively infinite volume of bulk soil whilst capturing at high precision any changes in the soil adjacent to the plant roots. In this case an effectively infinite volume of soil corresponds to any volume of soil which is sufficiently large that the phosphate depletion region about the root does not reach the edge of the domain considered. Using this model we are able to parameterize upscaled models for nutrient motion in soil ([Zygalakis et al., 2011](#_ENREF_33)).

This paper is arranged as follows: in section ‎2 we describe the plant growth, imaging and modelling approaches, in section ‎3 we discuss the results of numerical simulation and show how these models can be used to perform an image based study of root hair growth, finally in section ‎4 we discuss our results and show how these models might be further developed. The technical description of the mathematical models used in this paper is provided in appendix ‎A and appendix ‎B.

1. **Methods**
   1. **Plant growth**

We study a rice genotype Oryza Sativa cv. Varyla provided by the Japan International Research Centre for Agricultural Sciences (JIRCAS). The seeds were heat-treated at 50℃ for 48h to break dormancy and standardise germination. Germination was carried out at 23±1℃ for 2 days between moistened sheets of Millipore filter paper. The growth medium was a sand-textured Eutric Cambisol soil collected from a surface plot at Abergwyngregyn, North Wales (53o14’N, 4o01’W), the soil organic matter was 7%, full details are given in ([Lucas and Jones, 2006](#_ENREF_20)), soil B. The soil was sieved to <5 mm, autoclaved and air dried at 23±1℃ for 2 days. The dried soil was sieved to between bounds of 1680 μm and 1000 μm, producing a well-aggregated, textured growth medium.

Growth took place in a controlled growth environment (Fitotron SGR, Weiss-Gallenkamp, Loughborough, UK) for a period of 14 days. Growth conditions were 23±1℃ and 60 % humidity for 16 hours (day) and 18±1℃ and 55 % humidity for 8 hours (night) with both ramped over 30 minutes.

The seminal roots were guided by a specially designed growth environment fabricated in ABS plastic using an UP! 3D printer (PP3DP, China). The resulting assay is shown in Supplementary Figure 1 and further details are provided in ([Keyes et al., 2015](#_ENREF_18)) for details. The morphology of the growth environment was used to guide the roots into 7 syringe barrels (root chambers) which can then be detached for imaging once the growth stage is complete. The lower portion including the root chambers was housed in a foil-wrapped 50 ml centrifuge tube which occludes light during the growth period.

* 1. **Imaging**

Imaging of root chambers was conducted at the TOMCAT beamline on the X02DA port of the Swiss Light Source, a 3rd generation synchrotron at the Paul Scherrer Institute, Villigen, Switzerland. The imaging resolution was 1.2 μm, and a monochromatic beam was employed with an energy of 19 kV. A 90 ms exposure time was employed to collect 1601 projections over 180 degrees with a total scan time of 2.4 minutes. The data were reconstructed to 16-bit volumes using a custom back-projection algorithm implementing a Parzen filter. The resulting volume size was 2560x2560x2180 voxels.

The reconstructed volumes were analysed using a multi-pass approach ([Keyes et al., 2015](#_ENREF_18)). Whilst root hairs can be visualised in situ for dry soils they are challenging to distinguish from some background phases even at high resolution. Specifically, the portions of root hairs which traverse water filled regions of the pore space are indistinguishable from the water. The visible sections of the root hairs were extracted manually using a graphical input tablet (Cintiq 24, WACOM) and a software package that allowed interpolation between lofted cross-sections (Avizo FIRE 8, FEI Company, Oregon, USA). A number of these sections represent an incomplete root hair segmentation since proportions of the hair paths can be occluded by fluid rich phases and pore water. Full root hair paths were extrapolated from the segmented sections of partially visible hairs using an algorithm that simulates root hair growth ([Keyes et al., 2015](#_ENREF_18)). The algorithm was parameterised from the root hairs of plants (Oryza Sativa cv. Varyla) which were grown in rhizo-boxes with dimensions 30x30x2 cm, constructed of transparent polycarbonate with a removable front-plate, and wrapped in foil to occlude light. Hydration during the growth period was maintained via capillary rise from a tray of water, with occasional top-watering. The plants were grown in a glasshouse, with temperature ranging from 20-32 ℃ over the growth period. The root systems of 1 month old specimens were gently freed from soil using running water. One fine primary and one coarse primary were randomly sampled before manual removal of the remaining soil from the roots. Each was cut into a number of subsections of 2 cm length for analysis, each being imaged using an Olympus BX50 optical microscope. After stitching all images together 5 sub-regions were randomly defined for each section. Each region was chosen to represent a distance of 1 mm on the root surface. All hairs in sub-regions which were in sharp focus were measured in FIJI using a poly-line tool to generate a set of 220 hair lengths. A normal distribution was fitted to these data and used to parameterize the hair-growth algorithm. The fitted and sampled distributions are shown in Supplementary Figure 1. The mean of experimental lengths was 171.56 µm, compared to the mean fitted lengths: 173.67 µm. The standard deviation of the experimental lengths was 72.88 µm compared to the standard deviation of the fitted lengths 73.44 µm.

We observe that root hair density measured via Synchrotron Radiation X-ray CT data is generally slightly higher than for microscopy, probably due to the lack of damage artefacts. For the data in this study, the density is , compared to measured via bright-field microscopy in a study of similar rice varieties grown under similar conditions ([Wissuwa and Ae, 2001](#_ENREF_32)). This discrepancy is, in part, because the in situ hairs are often part-occluded by fluid and colloidal phases, it is usually only possible to obtain partial measurements in the Synchrotron CT data. This is offset to some degree by the lack of damage artefacts when compared to root-washing and microscopy, but the length values are low compared to most literature sources. However, in this study we explore the implications of soil domain size on nutrient uptake and have used hair data attained via quantification of soil-grown roots using bright field microscopy.

The root geometry was extracted in the same manner, manually defining the root cross-section from slices sampled (at a spacing of 120 µm) along the root growth axis. The soil minerals, pore gas and pore fluid were extracted using a trainable segmentation plugin in FIJI that implements the WEKA classifiers for feature detection using a range of local statistics as training parameters ([Hall et al., 2009](#_ENREF_12)).

The segmented geometry was used to produce 3D surface meshes, using the ScanIP software package (Simpleware Ltd., Exeter, United Kingdom). The root, hairs, gas fluid phase and soil minerals were exported as separate .STL files which provide the geometries on which the numerical models can be tested.

* 1. **Modelling**

We model the uptake of phosphate by a single root and root hairs in an unbounded partially saturated geometry, see Figure 1. In order to do this we extend the model described in ([Keyes et al., 2013](#_ENREF_17)). In ([Keyes et al., 2013](#_ENREF_17)) the authors considered a segment of root and surrounding soil. On the outer boundary of the segment a zero flux condition was applied. By definition this condition prevents any influx of nutrient from outside the domain considered. Hence, the total possible uptake is limited to the nutrient available from within the initial segment. This was adequate for the experimental situation considered, *i.e.*, a pot of radius *c.* , but is clearly not applicable for isolated roots in soil columns of radius larger than . We note that this is a slightly different scenario from the one studied by Barber ([Barber, 1984](#_ENREF_3)) in which the domain around the root was considered to be half the size of the inter-root spacing. In other words, Barbers model considered multiple roots effectively introducing root competition. In this work we consider a single isolated root and how that is affected by soil structural properties.

In order to overcome this limitation we consider a single root in a large/infinite domain of soil. However, as considering an infinite domain explicitly is computationally unfeasible, we break the domain into two regions: the rhizosphere and bulk soil. We assume that the bulk soil, which is far from the root, may be considered as a homogeneous medium with an effective phosphate diffusion constant. The effective diffusion properties of phosphate in the bulk soil are derived from the segmented CT data using the method of homogenization ([Pavliotis and Stuart, 2008](#_ENREF_24); [Zygalakis et al., 2011](#_ENREF_33); [Zygalakis and Roose, 2012](#_ENREF_34)). The nutrient flux in the bulk soil is then patched to the rhizosphere domain using a boundary condition which simulates an effective infinite region of bulk soil beyond the rhizosphere. In this section we introduce the equations and summarize the model which results from these assumptions. Full details of the derivation have been included in appendices ‎A and ‎B.

We assume that phosphate can only diffuse in the fluid domain, *i.e.*, no diffusion occurs in the air filled portion of the pore space. Therefore, we only present equations in the fluid region and its associated boundaries. However, we make no assumptions about the geometrical details regarding the air filled portion of pore space. If, from the CT data, there is air in contact with soil or root material this simply acts to reduce the surface area over which phosphate can be exchanged. We define two regions of fluid filled pore space we denote the rhizosphere by as the region explicitly considered near to the root. Physically we may think of this as an approximation to the rhizosphere. The second region is , the region of bulk soil outside of the rhizosphere, see Figure 2. As different boundary conditions need to be applied on each of the pore water interfaces we adopt the following naming convention. We take the interface between the two regions, located at a distance from the centre of the root to be . The root and root-hair surfaces are defined as , and respectively, the soil particle surface to be and in region and respectively. Finally we define the air water interfaces as and in region and respectively. The method we use to determine phosphate movement is different in each region. Phosphate movement in the rhizosphere is calculated based on a spatially explicit model obtained from CT data. Phosphate movement in the bulk soil is calculated analytically based on the solution to a spatially explicit numerical model in a representative volume of bulk soil. We present each of these models separately.

* + 1. **Rhizosphere**

In the rhizosphere we assume that phosphate moves by diffusion only

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| --- | --- | --- | --- |
|  |  |  | (1) |

where is the phosphate concentration in the soil solution and is the diffusion constant of phosphate in the soil solution. The phosphate is assumed to bind to the soil particles based on linear first order kinetics

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| --- | --- | --- | --- |
|  |  |  | (2) |
|  |  |  | (3) |

where and are the adsorption and desorption rates respectively, is the nutrient concentration on the soil surface and is the outward pointing surface normal vector. Here we have assumed that the nutrient concentration of the soil can be represented as a surface concentration and that any replenishment from within the soil aggregate is either so fast that it is captured by these equations or so slow that we can neglect it. We assume that there is no nutrient diffusion across the air water boundary

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (4) |

We consider uptake of phosphate from the fluid only. On the root surface this follows a linear uptake condition

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| --- | --- | --- | --- |
|  |  |  | (5) |

where is the nutrient uptake rate on the root and root-hair surfaces. For comparison with the paper by Keyes *et al* ([Keyes et al., 2013](#_ENREF_17)) we have chosen the absorbing power as , consistent with Nye and Tinker. Equation (5) is the small concentration equivalent of the Michaelis Menten condition, in which is the maximum rate of uptake and is the concentration when the uptake is half the maximum.

The flux on the root hair surface is given by one of two different scenarios: the first is linear uptake

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (6) |

The second case we consider is a pseudo time-dependent uptake which simulates linear uptake for a growing root-hair. We have termed this pseudo root-hair growth as we do not consider the geometrical and mechanical effects of root hair growth explicitly. Rather, we assume that at the root hairs are present, but do not contribute to uptake. As the simulation progresses the root hairs are assumed to grow at a certain rate. We model this by assuming an active region of root hair which grows outward from the root; this is illustrated in Figure 3. We write the root-hair uptake condition as

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| --- | --- | --- | --- |
|  |  |  | (7) |

where is the axial distance along the root hair, is the root hair growth rate, is an empirical parameter which controls the sharpness of the transition between the root hairs being “on”, *i.e.*, actively taking up nutrient and “off”, *i.e.*, not actively taking up nutrient.

The adsorption and desorption constants () are taken from ([Keyes et al., 2013](#_ENREF_17)) where they were derived using standard soil tests ([Giesler and Lundström, 1993](#_ENREF_10); [Murphy and Riley, 1962](#_ENREF_22)). The remaining parameters used in equations (1) to (5) were obtained from the literature ([Barber, 1984](#_ENREF_3); [Tinker and Nye, 2000](#_ENREF_27)) and are summarized in Table 1.

* + 1. **Rhizosphere bulk interface**

Due to the success of averaged equations in bulk soil, for example Darcy’s law and Richards’ equation ([Van Genuchten, 1980](#_ENREF_30)), the precise details of the geometry are less important in determining the total phosphate movement and average properties are sufficient to be considered. Therefore, rather than consider the explicit details of the geometry we derive an effective diffusion constant based on a representative soil volume in absence of roots. This is achieved using the method of homogenization, ([Pavliotis and Stuart, 2008](#_ENREF_24)), which is implemented as follows. First it is shown that, on the length scale of interest, the nutrient concentration is only weakly dependent on the precise structure of the soil. Secondly a set of equations, often called the cell problem, are derived which determine the local variation in concentration due to the representative soil volume. Finally an averaged equation is derived which describes the effective rate of diffusion in terms of an effective diffusion constant where is calculated from the bulk soil geometry (equations (A31) to (A34) and (A58)) and describes the impedance to diffusion offered by the soil. Full details of how is derived are provided in Appendix ‎A. Hence, in the bulk the diffusion of phosphate is described by

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| --- | --- | --- | --- |
|  |  |  | (8) |

where is the nutrient concentration in the bulk soil. The advantage of equation (8) is that we do not need to explicitly consider the soil geometry in the bulk soil domain. In itself this significantly reduces the computational cost for finite but large domains. However, rather than solving equation (8) numerically we find an approximate analytic solution for an infinite bulk soil domain subject to the conditions for and as . Using this solution we are able to define a relationship between concentration and flux at the edge of the rhizosphere. The result is a condition which simulates the presence of an infinite region of bulk soil at the rhizosphere soil domain boundary

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| --- | --- | --- | --- |
|  |  |  | (9) |

where is the Euler–Mascheroni constant. Hence, the bulk soil is dealt with entirely by condition (9). This significantly reduces the computational cost whilst allowing us to include the averaged geometric details of the bulk soil through the parameter . We note that the boundary condition (9) is singular at . This is regularized by the fact that when we have . To overcome the difficulties of implementing this we follow the suggestion of ([Roose et al., 2001](#_ENREF_25)) and modify equation (9) such that for small the equation is non-singular, see Appendix B. To summarise the final set of equations we solve in the rhizosphere are

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| --- | --- | --- |
|  |  | (10) |
|  |  | (11) |
|  |  | (12) |
|  |  | (13) |
|  |  | (14) |
|  | , | (15) |

where, in the linear uptake case, the root hair boundary condition is given by

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| --- | --- | --- |
|  |  | (16) |

In the root hair growth scenario the root hair boundary condition is given by

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| --- | --- | --- |
|  |  | (17) |

and is applied on the remaining external boundaries, see Figure 2. Equations (10) to (17) describe the uptake of phosphate by roots and root hairs from an infinite bulk of soil.

Using the STL files generated from the CT data a computational mesh is constructed using the snappyHexMesh package. The mesh is generated from a coarse hexahedral mesh and the STL surface meshes from the imaged geometry. The hexahedral mesh is shaped like a segment of initial angle , height and radius corresponding to the size of the domain to be modelled. Each of these parameters is increased until the root uptake properties converge. Successive mesh refinements are made where the mesh intersects any geometrical feature described by the STL files, *i.e*., the mesh is refined about the surfaces of interest. Once the mesh has been refined to hexahedra of side length less than 1 about the STL surfaces the regions outside of the water domain are removed. The remaining mesh is then deformed to match to the STL surfaces. Finally the mesh is smoothed to produce a high quality mesh on which the numerical models can be run. The equations are discretised on the mesh and solved in OpenFOAM, an open source finite volume code ([Jasak et al., 2013](#_ENREF_16)), using a modified version of the inbuilt LaplacianFOAM solver to couple the bulk concentration to the sorbed concentration at the soil boundaries. Time stepping is achieved using an implicit Euler method with a variable time stepping algorithm for speed and accuracy. All numerical solutions were obtained using the Iridis 4 supercomputing cluster at the University of Southampton.

1. **Results and discussion**

Using the theory developed in section ‎2.3 we calculate the bulk soil effective diffusion constant and nutrient uptake properties of a single root with hairs. We consider two different water contents. The first of which is the case in which all the pore space is full of water, *i.e.*, where is the volumetric water content defined as the volume of water divided by the volume of pore space. Secondly we use the segmented CT image to obtain the water content and air-water interface from the scanned soil. In this case the volumetric water content is . In addition to being able to parametrize existing models we also calculate the size of the region which needs to be considered for the uptake predicted by our simulations to converge. Finally we consider how a growing root-hair system affects the overall uptake properties of the root and root-hairs.

* 1. **Bulk soil properties**

Before we consider the nutrient uptake properties of the plant root system we first find the homogenized properties of the bulk soil. From the CT image, Figure 1, we select a cube of soil of side length . From this we sub sample a series of geometries of size for , *i.e.*, we repeatedly half the volume of bulk soil considered, and solve equations (A31) to (A34) and (A58) to obtain . The key difficulty that arises in solving these equations is that they require the geometry to be periodic, *i.e*, it is composed of regularly repeating units. In reality this is not the case. Hence, we have to impose periodicity. Following the method used in ([Tracy et al., 2015](#_ENREF_28)) we impose periodicity by reflecting the geometry about the three coordinate axes. We note that this reflection is achieved mathematically through analysis of the symmetries of the problem rather than by physically copying the meshes. This is discussed in more detail in the appendix and results in solving equations (A35) to (A39). Computational resources ranged from 46 Gb across 2 nodes for 3 minutes for Saturated case with to 900Gb across 16 nodes for 45 minutes for the more complex partially saturated case with . As we increase the size of we find that the value of converges to a fixed value once a sufficiently large sub sample volume is included. Figure 4 shows these values for saturated and partially saturated soil. We see that for small the effective diffusion coefficient is a function of . However, as is increased the value is seen to level off and become effectively independent of our choice of . We interpret this to mean that has converged and will not change if is increased further. As a measure of convergence we assume that has converged if doubling the volume of soil considered, corresponding to increasing by 1, causes a change in which is smaller than 5% of its final value. The effective diffusion constant returns a converged value for , corresponding to =0.63 mm, see Figure 4. However, due to the symmetry reduction used in deriving equations (A35) to (A39) this side length must be doubled to obtain the true representative volume. Hence, the actual size of the representative volume is =1.26 mm. At this value the computational resources used were 75Gb across 2 nodes for 45 minutes in the saturated case and 150 Gb across 4 nodes for 7 minutes in the partially saturated case. The larger resource requirements are necessary for the partially saturated case due to the increased resolution needed to capture thin water films. We note that, although a representative side length of =1.26 mm may seem small the soils used here were sieved to between two relatively close tolerances 1.00 and 1.68 mm. Hence, these soils will be very homogeneous and we would expect the final soil packing to be close to an ideal sphere packing. The value of is seen to converge to for the saturated soil and for the partially saturated soil. No data is plotted for the partially saturated case with because, for samples this small, the air films and soil provided a complete barrier to diffusion and no effective diffusion coefficient could be calculated.

* 1. **Nutrient uptake properties**

Using the values obtained for at full and partial saturation we now consider the uptake of nutrient by the plant root system shown in Figure 4. We are interested in finding the size of the volume of soil about the root which we need to consider geometry explicitly in order to accurately represent the uptake of phosphate by the root and root hairs. To determine the size of this volume we consider a segment of angle , height and radius centred on the root. The maximum radius considered is , and . The height, radius and angle of the segment considered are increased from 20% of the maximum domain size in steps of 20% till the maximum is reached corresponding to a total of 125 simulations for each of the saturated and partially saturated cases. Computational requirements ranged from 15 Gb across 2 nodes for 15 minutes in the simplest case to 300 Gb across 12 nodes for 16 hours in the most complex case.

Typical plots for the nutrient movement in the saturated and partially saturated cases are shown in Figure 5 for a variety of values with the smallest and values used. Initially we expected that there would be two convergence criteria; firstly a sufficiently large root surface area will need to be considered in order for the number of root hairs involved in nutrient uptake to be representative, *i.e.*, the density of root hairs in the sub volume is equal to the density of root measured density of root hairs. Secondly the radius of the region considered must be sufficiently large that all the rhizosphere soil is captured. However, whilst there is some variance in the data with root surface area, Figure 7 and error bars in Figure 6, it seems that the main convergence criteria is that a sufficiently large value of , i.e., the location of the outer rhizosphere-bulk soil boundary, is used. Whilst this conclusion is somewhat surprising it seems that only a relatively small value for and are required to capture enough of the root hair structure that it is representative. On inspection we see that the ratio between the root hair area and root area quickly settles to for root hair surface areas greater than . Hence, for root surfaces areas above this value the effective density of root hair surface area does not change and the uptake properties are not expected to change significantly.

To check the convergence of the simulated phosphorous dynamics we compare the total flux at the root and root hair surfaces as a function of time for the linear uptake conditions. These data are presented in Figure 6 for both saturated and partially saturated conditions for the root uptake and Figure 7 for the root-hair uptake. The simulated nutrient uptake is seen to settle to a rate which is independent of for sufficiently large . We assume that the total uptake has converged once increasing produces a change in uptake of less than 5% of the final value. The radius at which this is seen to occur is for the saturated case and for the partially saturated case. In the saturated case at the cumulative uptake of the root and root hair surfaces is , this converges to for . In the partially saturated case the cumulative uptake at is This converges to for . It is interesting at this point to compare our model with the zero flux approximation used in ([Keyes et al., 2013](#_ENREF_17)). In this case the total uptake can easily be calculated as the total amount of phosphate available in the geometry at time . For the largest saturated domain we have considered this would be a total uptake of , which is significantly less than the uptake measured here (). We note that the uptake by the root hairs converges in a diminishing oscillatory manner, *i.e.*, the uptake first increase with before decaying to a steady state. This is because at the smallest value of the geometry does not contain the entire length of the root hairs. Hence, the root hair uptake is noticeably lower than the cases . Once the full hair length is taken into account the convergence is smooth and behaves the same way as the convergence of the root uptake.

As with the effective diffusion constant we find that we do not need to consider a large amount of soil in order to obtain converged properties. Hence, we can observe that the radius required to capture the behaviour of the rhizosphere was dependent on the saturation of the fluid. In the fully saturated case the radius simply needed to be large enough to slightly greater than 100% of the root hair length, *i.e.*, 1.1 mm. However, in the partially saturated case a much larger radius (roughly double the root hair length) was required to capture the corresponding effect on the nutrient motion. We observe that if we using this model we can parameterise mathematically simpler models such as the one developed in ([Roose et al., 2001](#_ENREF_25)). By using the effective diffusion constant and additional uptake provided by the root hairs to parameterize the model in ([Roose et al., 2001](#_ENREF_25)) we obtain a cumulative uptake of using   and for the uptake parameter in the saturated case. In the partially saturated case we obtain a cumulative uptake of 31.2 using   and . In both cases the model developed by Roose can be agrees well with our predictions assuming the effective uptake parameter is a function of saturation. In the fully saturated case the root hairs offer an increase in uptake of 30%. In the partially saturated case the effective uptake is decreased. This is in part due to the decrease in root and root hair surface area which is in contact with water, 80% compared to the fully saturated case. Hence, whilst the root hairs considered in this geometry do increase root uptake when comparing image based simulations, they do not significantly alter the uptake parameters in the conventional models.

* 1. **Root hair growth**

We now consider the root hair growth scenario. We neglect the geometrical growth of the root hairs and consider a growing region on which uptake occurs. We use a representative set of values for , and for which the simulation has converged. Specifically we take, and for the fully saturated case and , and for the partially saturated case. The root hair growth is shown schematically in Figure 8 for a range of different times. The hair growth parameter is chosen to give the root hairs an effective growth period of two days and the empirical parameter is chosen such that the , *i.e.*, the distance between the active and non-active sections of the root hair is of length . Alongside the uptake results for the saturated and partially saturated cases, shown in Figure 9, we have plotted the uptake results for the standard fixed root hairs case. Interestingly, other than the magnitude of the flux, there is little qualitative difference between the saturated and partially saturated cases.

The main difference between the root hair growth and the static root hair scenario is observed towards the start of the growth period, between 0 and 48 hours. In the growth scenario, as expected, the uptake is dominated by the root for short times. However, as time progresses the root-hairs grow and provide the dominant contribution to nutrient uptake. Once the nutrients in the region immediately adjacent to the root have been taken up the uptake in the growing root hair quickly settles to match the uptake rate for the fixed root hair case. After 48 hours have passed and the root hairs are fully developed the fixed and growing root hair scenarios have identical uptake power. Hence, after 48 hours, the difference in cumulative uptake between the two scenarios is less than 1%. This suggests that the fixed root hair provides a good approximation for nutrient uptake and that more detailed modelling of root hair growth may not be necessary for timescales longer than 48 hours and shorter than the root hair lifetime.

1. **Conclusions**

In this paper we have extended the image based modelling in ([Keyes et al., 2013](#_ENREF_17)) to consider large/infinite volume of soil around the single hairy root. The bulk soil properties are captured from an X-ray CT image based geometry using the method of homogenization to transform the imaged geometry into a homogeneous medium with an effective diffusion constant based on the geometrical impedance offered by the soil. The bulk soil region is then patched onto the rhizosphere using a boundary condition which relates the concentration at the surface of the rhizosphere to the flux into the rhizosphere. The advantage to image based modelling of this type is that it can be used to answer specific questions on the movement of nutrient based on the soil geometry and root hair morphology. This information can then be used to parameterise simplified models and gain understanding of rhizosphere processes.

The method is tested for two different soil water saturation values by considering bulk and rhizosphere soil samples of different sizes which are increased until the effective transport and uptake properties of the two regions are seen to converge. We found that the key criterion for convergence of nutrient uptake simulations is that a sufficiently large radius of soil about the root is considered. However, we emphasize that this is likely to be dependent on root hair morphology, moisture content and soil type. Hence, convergence checks should be carried out on a smaller scale for different geometries. It is interesting to note that the radius of the segment about the root needed for convergence to occur is dependent on the saturation considered. Specifically we need to consider a larger region of soil about the root for lower saturation values 1.4 mm of soil compared to the 1.1 mm of soil for the saturated case. This observation is attributed to chemical effects present in the rhizosphere which cause variation in the fluid properties ([Gregory, 2006](#_ENREF_11)). In our CT scans these changes would be picked up as a geometrical variation either in the fluid location or the contact angle at the air water interface. Hence, in the fully saturated case we would not see these effects as the specific water location is neglected. By dividing the CT image into regions , , , and and calculating the saturation in each case we see a noticeable decrease in saturation for , ( compared to for all other regions). Therefore, in order to capture the geometric impedance created by this region we require .

In agreement with the paper by ([Keyes et al., 2013](#_ENREF_17)) we can observe that in both cases the root hairs contribute less than the root surfaces to the nutrient uptake. However, this difference is small and, in terms of order of magnitude, both the hairs and the roots contribute equally to the nutrient uptake. A major advantage to this type of modelling is that these simulations can be used to parameterise existing models which may be computationally less challenging, for example the one in ([Roose et al., 2001](#_ENREF_25)). In this case we see that the root hairs contribute approximately an extra 30% to the root uptake, an important consideration which will increase the predictive ability of the model developed in ([Roose et al., 2001](#_ENREF_25)). Again, it may be that in poorly saturated soils, *i.e.*, those with much lower moisture content than the 33%, there will be less water in contact with the root and the root hairs, which can penetrate into the smaller pores within the soil, may provide a more significant contribution. Further investigation across a range of saturation values either based on imaging of samples at different water content, or application of a spatially explicit moisture content model such as the one developed in ([Daly and Roose, 2015](#_ENREF_5)), would be needed to verify this.

Using the minimum value of *,*  and obtained for the two cases we have considered the effect of pseudo root-hair growth on nutrient uptake neglecting the geometrical and mechanical effects of root-hair growth. As the non-active root hairs are still geometrically represented in the domain they may act to weakly impede the diffusion from the soil into the root itself. The root hair growth modelling showed that, although there are differences in the ratio of root and hair uptake rates towards the start of the growth period, *i.e.*, two days. However, on the long timescale, *i.e.*, times larger than two days, the rate of uptake is unaffected by the growing root hairs, see Figure 9. This suggests that more detailed modelling of the root hair growth might not yield different results and the fixed root hair approximation may provide a detailed enough picture for further investigation into the effects of root hairs.

The method developed here provides a powerful framework to study properties of the rhizosphere. We have tested the model for a specific geometry obtained from X-ray CT, however we emphasise that the results obtained are suggestive of certain trends they will be dependent on the precise soil type, water content and root hair morphology studied. Hence, studying different root hair distributions and soil structures will allow a greater understanding of how root hairs uptake nutrients to be developed. Further development of this method to couple a spatially explicit water model to the nutrient uptake will allow similar understanding to be developed for water distribution and uptake.

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**Data Accessibility**

All reconstructed scan data will be available on request by emailing [krd103@soton.ac.uk](mailto:krd103@soton.ac.uk)

1. **Diffusion in bulk soil**

As in the rhizosphere transport is assumed to be by diffusion only

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A1) |

where is the phosphate concentration in the soil solution for the bulk soil. We assume that the concentration and concentration flux are continuous across the rhizosphere-bulk soil boundary

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A2) |
|  |  |  | (A3) |

and consider a linear reaction on the soil surface

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A4) |
|  |  |  | (A5) |

and zero flux on the air water boundary

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A6) |

In keeping with ([Keyes et al., 2013](#_ENREF_17)) we non-dimensionalize with the following variables: , , , , (for all lengths) and use , , and to obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A7) |
|  |  |  | (A8) |
|  |  |  | (A9) |
|  |  |  | (A10) |
|  |  |  | (A11) |
|  |  |  | (A12) |

Here , , , and are summarized in Table 2 and is a typical length scale of the domain we are interested in. Throughout this paper we take m, i.e. the average radius of the rice/wheat/corn fine roots.

Before we derive the boundary condition we consider the homogenization problem in the bulk soil. The key assumption of the homogenization method is that the two length scales, and , may be dealt with independently. Therefore, we can expand the vector gradient operator as **,** where and are the vector gradient operators on the scale and respectively, , corresponding to . We also define the concentrations in terms of an expansion of the form

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A13) |
|  |  |  | (A14) |

Physically and can be thought of as the average concentrations on the soil surface and in the solution within the bulk soil domain. The remaining parameters and are corrections to the average concentration which capture small scale variations within the soil and the effects of the linear reactions on the soil surface. We rescale time to capture diffusion over the distance  *(,*  and ) and obtain the scaled equations in the bulk soil

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A15) |
|  |  |  | (A16) |
|  |  |  | (A17) |
|  |  |  | (A18) |
|  | periodic in |  | (A19) |

Substituting equations (A and (A14) into equation (A15) to (A19) and collecting terms in ascending orders of we obtain a cascade of problems for and .

* 1. :

The equations at are

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A20) |
|  |  |  | (A21) |
|  |  |  | (A22) |
|  |  |  | (A23) |
|  | periodic in |  | (A24) |

which have solution . Hence, on the timescale of diffusion the linear reactions have already happened and the surface concentration and the bulk concentration are equal and the leading order concentration is independent of the microscale structure.

* 1. :

Expanding to and using the results from the expansion we obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A25) |
|  |  |  | (A26) |
|  |  |  | (A27) |
|  |  |  | (A28) |
|  | periodic in . |  | (A29) |

This is the standard correction to a diffusion only problem, it has solution , where is a function of only which will be defined at higher order and

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A30) |

and satisfies the cell problem

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A31) |
|  |  |  | (A32) |
|  |  |  | (A33) |
|  | periodic in |  | (A34) |

Equations (A31) to (A40) assume that the soil sample is geometrically periodic, *i.e.*, it is composed of regularly repeating units. In reality this is not the case so these equations cannot directly be applied. To overcome this we impose a mathematical periodicity by reflecting the geometry along the three coordinate axes. Reflecting about the -th coordinate axis using the substitution in equations (A31) to (A40) we observe that, in order for the equations to remain unchanged, we must have . Similarly by reflecting about the -th coordinate axis using the substitution ,for in equations (A31) to (A40) we see the equations remain unchanged. Hence we infer that is odd when reflected about the -th coordinate axis and even otherwise. As a result we are able to solve a set of equations on the original domain which respect these symmetries

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A35) |
|  |  |  | (A36) |
|  |  |  | (A37) |
|  | = 0 |  | (A38) |
|  | = 0 |  | (A39) |

A direct result of this analysis is that the dimensional volume used in equations (A35) to (A39) represents one eighth of the total representative volume as the total volume can be reconstructed by mirroring the result along the three axes.

* 1. :

Expanding to and using the previous solutions we obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A40) |
|  |  |  | (A41) |
|  |  |  | (A42) |
|  |  |  | (A43) |
|  | periodic in |  | (A44) |

Before we solve for and we require that a solution exists. Integrating and using the divergence theorem we obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A45) |

where . As in the case we obtain a cell problem for and . , where is an arbitrary function of which will be defined at higher order and

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A46) |

Here satisfies

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A47) |
|  |  |  | (A48) |
|  |  |  | (A49) |
|  | periodic in |  | (A50) |

and we have already solved the cell problem for .

* 1. :

In order to capture the effect of the linear reaction on the soil surface we expand to to obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A51) |
|  |  |  | (A52) |
|  |  |  | (A53) |
|  |  |  | (A54) |
|  | periodic in |  | (A55) |

Applying the solvability condition and using the results from previous expansions we find

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A56) |

where . By writing we can combine the results at and to obtain

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A57) |

where we have neglected terms . The effective parameters in equation (A57) are

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A58) |

and

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (A59) |

Note, we have added terms at to simplify the form of the final equation. The can be formally calculated by expanding to . However, as we are only really interested in knowing the approximate averaged behaviour of diffusion in the soil we neglect the final term in equation (A57).

1. **Resupply boundary condition**

We assume that equation (A57) is valid far from the root and root hair. We now consider an infinite volume of soil surrounding the root and derive an approximate boundary “resupply” condition at the interface between the Rhizosphere and Bulk soil regions to capture the influx of nutrient from outside the explicit domain of interest. We assume that the main direction of diffusion is towards the root. Hence, we can reduce the diffusion equation far from the root to a one spatial dimension equation with an isotropic diffusion constant . In the bulk soil we consider the radial diffusion equation

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B1) |

subject to the boundary conditions

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B2) |

and

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B3) |

We add the condition that . We follow the approach of ([Roose et al., 2001](#_ENREF_25)) and solve equation (B1) in regions close to the root and far from the root. Matching these solutions together at we derive an expression for the flux into the rhizosphere. We assume that, near the rhizosphere boundary, *i.e.*, the concentration will approximately be given by the steady state solution

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B4) |

where is an arbitrary constant and is the, as yet undefined, flux into the rhizosphere. Far from the rhizosphere we use the similarity solution, see for example ([King et al., 2003](#_ENREF_19); [Roose et al., 2001](#_ENREF_25)),

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B5) |

where is the exponential integral. By equating equations (B4) and (B5) at and assuming continuity of concentration on the rhizosphere-bulk soil boundary we find

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B6) |

where is the Euler–Mascheroni constant. We note that in deriving equation (B6) we have implicitly assumed that does not vary significantly with time. The logarithm in the denominator of equation (B6) is singular at , hence, for numerical stability we modify the equation slightly. This approach means that the boundary condition is not accurate for small time. However, the timescale over which this occurs is short and the effect on the uptake properties is small. Following the method of ([Roose et al., 2001](#_ENREF_25)) we modify equation (B6) such that at ,

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  | (B7) |

Equation (B7) is used to parameterize the bulk soil and feeds directly into the model for nutrient movement in the rhizosphere in the main body of the paper.

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|  |  |  |  |
| --- | --- | --- | --- |
| **Constant** | **Value** | **Units** | **Description** |
|  |  |  | Diffusion constant |
|  |  |  | Uptake constant |
|  |  |  | Uptake rate |
|  |  |  | Desorption rate |
|  |  |  | Adsorption rate |
|  |  |  | Root hair growth rate |
|  |  |  | Root hair cut off rate |

Table : Physical parameters used in nutrient model.

|  |  |  |  |
| --- | --- | --- | --- |
| **Parameter** | **Expression** | **Values** | **Description** |
|  |  |  | Dimensionless flux coefficient |
|  |  |  | Dimensionless desorption rate |
|  |  |  | Dimensionless uptake rate |
|  |  |  | Dimensionless root hair growth rate |
|  |  |  | Dimensionless root hair cut off rate |

Table 2: Dimensionless parameters used in rescaled diffusion model.

**Figure captions**

Figure : Image based geometry: (A) X-ray CT image of the roots, root hairs, soil and pore water. (B) shows one of the rhizosphere segments considered with size described by the angle , height h and radius r. (C) shows a cube of bulk soil of side length L.

Figure : Schematic of the different regions used in the mathematical formulation of the problem. The bulk and rhizosphere regions are highlighted with the modelling domains , , , , and labeled for the rhizosphere and , and labeled for the bulk soil.

Figure 3: Schematic for root hair growth. The root hair geometry remains unchanged throughout the simulation. As the simulation progresses the active portion of the root hair grows. The streamlines show an estimation of the nutrient transport as affected by the presence of the root hair. At t=0 the root hair is non-active and acts only to geometrically impede the transport of nutrient. At t=1 day the root hair has grown to half its final length and acts partly to take up nutrients and partly as a geometrical impedance. Finally at t=2 days the root hair is fully grown.

Figure 4: Effective diffusion coefficient as a function of L , the side length of the cube. The results are plotted for the saturated case, S=1, corresponding to the pore space being completely full of water and partially saturated, S=0.33, corresponding to 1/3 of the pore space being occupied by water. As L is increased the saturated and unsaturated effective diffusion properties are seen to converge to a steady value corresponding to the bulk diffusion coefficient.

Figure 5: Typical plots obtained from simulation for, (1A) to (1E). the saturated case and, (2A) to (2E), the partially saturated case. The five images in each case correspond to and for (A) , (B) , (C) , (D) and (E) . The streamlines show the effective diffusion paths with red corresponding to high nutrient concentration and blue corresponding to lower nutrient concentration.

Figure 6: Log-linear plot of flux into (A) the root hairs in the saturated case, (B) the roots in the saturated case, (C) the root hairs in the unsaturated case and (D) the roots in the unsaturated case. The lines show the average flux over a period of one week for the five different radii considered up to a maximum of r\_max=1.76 mm. As r is increased the uptake profile is seen to converge. The figure insets show a zoomed in section of the same curve with error bars removed for clarity.

Figure 7: Total uptake into the root and root hair system averaged over all time points. Plot shows average uptake over the different radii considered with standard deviation error bars as a function of root surface area.

Figure 8: Root growth scenario for four different times: The top left shows the initial condition ( 0 hours), the top right shows the hair growth after 16 hours, the bottom left shows hair growth after 32 hours and the bottom right shows hair growth after 48 hours.

Figure 9: Flux at the root and hair surfaces for the root growth scenario in comparison to the fixed root hair scenario for the saturated and partially saturated geometries (logarithmic scale). The combined uptake of the root and hair is also plotted.