



Upscaling from rhizosphere to whole root system: Modelling the effects of phospholipid surfactants on water and nutrient uptake

Vanessa M. Dunbabin^{1,3}, Sean McDermott² & A. Glyn Bengough²

¹Tasmanian Institute of Agricultural Research, University of Tasmania, Private Bag 54, 7001, Hobart, Tasmania, Australia. ²Scottish Crop Research Institute, Invergowrie, DD2 5DA, Dundee, Scotland.

³Corresponding author*

Received 28 October 2004. Accepted in revised form 18 January 2005

Key words: lecithin, nutrient availability, phosphate, root architecture, root mucilage, wheat

Abstract

While the rhizosphere presents a different chemical, physical and biological environment to bulk soil, most experimental and modelling investigations of plant growth and productivity are based on bulk soil parameters. In this study, water and nutrient acquisition by wheat (*Triticum aestivum* L.) roots was investigated using rhizosphere- and root-system-scale modelling. The physical and chemical properties of rhizosphere soil could be influenced by phospholipid surfactants in the root mucilage. Two models were compared: a 2-dimensional (2D) Finite Element Method rhizosphere model, and a 3-dimensional (3D) root architecture model, ROOTMAP. ROOTMAP was parameterised to reproduce the results of the detailed 2D model, and was modified to include a rhizosphere soil volume. Lecithin (a phospholipid surfactant) could be exuded into the rhizosphere soil volume, decreasing soil water content and hydraulic conductivity at any given soil water potential, and decreasing phosphate adsorption to soil particles. The rhizosphere-scale modelling ($5 \times 5 \text{ mm}^2$ soil area, 10 mm root length, uptake over 12 h) predicted a reduction in water uptake (up to 16% at 30 kPa) and an increase in phosphate uptake (up to 4%) with lecithin exudation into the rhizosphere, but little effect on nitrate uptake, with only a small reduction in dry soil (1.6% at 200 kPa). The 3D root model reproduced the water ($y = 1.013x$, $R^2 = 0.996$), nitrate ($y = 1x$, $R^2 = 1$) and phosphate ($y = 0.978x$, $R^2 = 0.998$) uptake predictions of the rhizosphere model, providing confidence that a whole root system model could reproduce the dynamics simulated by a Finite Element Method rhizosphere model. The 3D root architecture model was then used to scale-up the rhizosphere dynamics, simulating the effect of lecithin exudation on water, nitrate and phosphate acquisition by a wheat root system, growing over 41 d. When applied to growing and responsive roots, lecithin exudation increased P acquisition by up to 13% in nutrient-rich, and 49% in relatively nutrient-poor soil. A comparison of wheat (*Triticum aestivum* L.) and lupin (*Lupinus angustifolius* L.) root architectures, suggested an interaction between the P acquisition benefit of rhizosphere lecithin and root architecture, with the more highly-branched wheat root structure acquiring relatively more P in the presence of lecithin than the sparsely-branched lupin root system.

Introduction

The rhizosphere is not only different chemically, physically and biologically from bulk soil (Bowen and Rovira, 1999), but the processes that drive

this difference are complex and spatially and temporally dynamic. Root architecture and physiology, root-induced changes in water and nutrient availability, root exudates, and fungal and bacterial associations (e.g. McCully, 1999; Hinsinger, 2001; Kirk, 2001; Neumann and Römheld, 2002; Gahoonia and Nielsen, 2004), are all components of the dynamic rhizosphere system. While the

* FAX No: +61 3 6226 2651

E-mail: Vanessa.Dunbabin@utas.edu.au

understanding of many of the individual components of the rhizosphere is increasing, the integration of these components and upscaling to whole-plants, crops and ecosystems, is an area of rhizosphere research that is in its infancy. The ability to integrate rhizosphere processes is important for determining the impact of rhizosphere-scale interactions on plant and crop productivity.

Plant and crop models are tools that can play a role in integrating rhizosphere processes and investigating their relative impact at plant and crop scales. To date, most plant and crop models have been based on bulk soil parameters, often incorporating numerical schemes for deducing nutrient concentrations at root surfaces from bulk soil parameters (e.g. Baldwin et al., 1973; Darrah and Roose, 2001; Roose and Fowler, 2004), but not explicitly representing the rhizosphere as a volume of soil with properties that can be substantially different from those of the bulk soil.

While a number of models have been developed for investigating rhizosphere processes at the rhizosphere-scale (e.g. Darrah, 1996; Jones et al., 1996; Calba et al., 1999; Toal et al., 2000; Kirk, 2002a, b), there is a need to incorporate rhizosphere-scale interactions into plant and crop models. Factors such as 2- and 3-dimensional (2D and 3D) spatial heterogeneity, temporal dynamics (daily to seasonal scale), crop architecture and crop agronomy could then be considered, allowing the influence of rhizosphere processes to be investigated in the context of other agronomic factors. Toal et al. (2000) discuss how current rhizosphere carbon flow models do not consider the consequences of highly overlapping and interacting rhizospheres, characteristic in the topsoil of some agronomic and natural systems. Toal et al. (2000) suggest that 3D root architectural models could be used to generate realistic rhizosphere maps for input into rhizosphere carbon flow models. In a rare example, Arah (2001) included a rhizosphere compartment into a model of irrigated rice crops. The capacity to reproduce the process dynamics contributing to CH₄ emission from rice crops, improved when the rhizosphere compartment was included.

In this study, we used a Finite Element Method water and solute transport model (based on Huang et al., 1998), to investigate root water, nitrate and phosphate acquisition at the rhizo-

sphere-scale. In these simulations soil properties, out to 1 mm from the root surface, could be affected by lecithin, an analogue for the phospholipid surfactants present in maize, lupin and wheat root mucilage (Read et al., 2003). Lecithin has been found to change the water release and phosphate adsorption properties of soil (Read et al., 2003). These simulations were designed to investigate the effect of these changes in rhizosphere soil properties, on water and nutrient acquisition by plant roots.

A 3D root architecture model, ROOTMAP (Diggle, 1988; Dunbabin et al., 2002), was used to scale-up the dynamics predicted from the rhizosphere-scale modelling, to the root-system-scale. The ROOTMAP model was initially parameterised to reproduce the output from the Finite Element Method model. ROOTMAP was then used to simulate water, nitrate and phosphate uptake by a growing and responsive 3D wheat root architecture, to investigate the interaction between root architectural dynamics, the presence of lecithin in rhizosphere soil, and resource acquisition. A comparison between the architecturally distinct wheat and lupin root systems was also made.

Materials and methods

The effect of lecithin on soil water release and P adsorption

In an earlier study, Read et al. (2003) analysed the phospholipid surfactant content of maize (*Zea mays* L. cv. Freya), lupin (*Lupinus angustifolius* L. cv. Merrit) and wheat (*Triticum aestivum* L. cv. Charger) root mucilage. The lipids present in the mucilage were principally phosphatidylcholines. Read et al. (2003) identified a commercially available phosphatidylcholine surfactant, (soybean) lecithin, which had comparable properties to the measured lipids. Lecithin was used to test the effect of the phosphatidylcholine content of root mucilage on the water release and phosphate adsorption properties of soil. When applied to a dark-brown sandy loam (Bullionfield Soil, strong phosphate adsorber), lecithin reduced soil water content at all water tensions (over a range of 0.5–1500 kPa), with the greatest reduction in water content (up to 10%)

at low tension (0.5–17 kPa) (Read et al., 2003). Lecithin decreased hydraulic conductivity in the rhizosphere by causing larger water-filled pores to drain. Hydraulic conductivity was reduced by 68–78% over the soil water tension range focussed on in this current study (30–200 kPa). Lecithin reduced phosphate adsorption to soil, increasing the proportion of P in the solution phase. Lecithin also reduced the rate of N mineralisation in soil, possibly through a direct effect on the microbial population, or as a consequence of the changed moisture release and P adsorption characteristics of the soil (Read et al., 2003).

2D finite element method model – rhizosphere-scale modelling

The rhizosphere-scale modelling was carried out using a Finite Element Method (FEM) model designed to simulate non-linear soil water flow and reactive solute transport to cylindrical roots in 2D unsaturated soil. The model is based on a mass-conservative Picard iterative scheme (Huang et al., 1998). It incorporates Richard's equation for soil water flow, the advection-dispersion equation for solute transport, and van Genuchten's (1980) relationships for soil water retention and conductivity (Eqs. 1, 2; see Appendix 1 for equations). Nutrient uptake from grid cells adjacent to the root surface is calculated using the Michaelis–Menten kinetic function (Eq. 3), and water uptake at the root surface is a function of the soil water potential and the hydraulic resistance of the plant (Eq. 4). The Langmuir equation was used to describe the phosphate adsorption isotherms (Eq. 5). The model is coded in Salford Fortran, with visualisation routines in C⁺⁺ and Mathematica.

3D root architecture model, ROOTMAP – whole root system modelling

The ROOTMAP three-dimensional root architecture model is described in detail in Diggle (1988) and Dunbabin et al. (2002). Briefly, the model considers soil water and nutrient dynamics, and root growth responses to these dynamics. Solute transport is described by the advection-dispersion equation. Solute concentration at the root surface is derived from local bulk-soil values (which vary in 3D space depending upon the grid resolution) using the Baldwin et al. (1973) model (Eq. 6).

This model uses Michaelis–Menten kinetics to describe plant capacity to take up ions present at the root surface (Eq. 3). In this rhizosphere version of the model, water and nutrients are transported between the bulk soil and rhizosphere soil by mass flow and diffusion. Solute and water uptake is from the rhizosphere soil volume, and solute concentrations at the root surface are derived from the average rhizosphere concentration, using Eq (6). The water uptake routine is based on the Feddes sink term (Eq. 7; Feddes et al., 1976). The redistribution of water in 3D space is described by Darcy's law (Eq. 8).

ROOTMAP utilises a positive feedback relationship between plant demand signals for each simulated soil resource (water, nitrate and phosphate in these simulations), and local supply signals from each root segment. The interaction of the supply/demand signals drives the allocation of internal assimilates, affecting growth rate of root tips, root branching behaviour, and local nutrient uptake rates, reproducing the feedback control systems thought to operate in plants (Clarkson and Lüttge, 1991; King et al., 1993; Zhang and Forde, 1998). Each additional unit of nutrient that the simulated plant obtains, enables it to generate further assimilates for future growth. This is a positive feedback relationship, so that proliferation of roots in local nutrient patches will be greater when the plant demand for the nutrient is high, compared to when plant demand is low.

In order to replicate the behaviour of the Finite Element Method model (described above) van Genuchten's (1980) relationships were included in ROOTMAP for describing soil water retention and conductivity (Eqs. 1, 2), and the Langmuir equation was used to describe the phosphate adsorption isotherms (Eq. 5).

Model parameterisation

As described above, Read et al. (2003) measured the effect of lecithin on the water release and phosphate adsorption characteristics of Bullionfield soil. The van Genuchten (1980) expression for soil water retention (Eq. 1), and the Langmuir expression for phosphate adsorption (Eq. 5) were fitted to these experimental data, enabling the two models to replicate the water release and phosphate adsorption isotherm characteristics of Bullionfield soil, with and without lecithin present.

In order to replicate the water uptake behaviour of the Finite Element Method model, the weighting function for water uptake $\alpha_w(\psi)$ in ROOTMAP (Eq. 7) was scaled using the fitted water release function (Figures 1a, 2). This weighting function describes the ability of the plant to extract water from the soil profile as a function of soil water potential (Feddes et al., 1976).

The ROOTMAP model was modified to include a rhizosphere soil volume, distinct from the bulk soil volume. As a root system develops, the model tracks the development of the rhizosphere in 3D space. For these simulations, the rhizosphere was defined (in both models) as 1 mm thick. Lecithin has only recently been identified in root exudates (Read et al., 2003), with no published data on its spatial distribution in the rhizosphere. Rhizospheres have been estimated to range from 0.5 to 2.0 mm in radius for a range of species (Toal et al., 2000). Using a root radius of 0.2 mm (in the 12 h simulations) and a rhizosphere thickness of 1 mm gives a rhizosphere radius (1.2 mm) at about the mid-point of the reported range. Lecithin was assumed to be present in the whole rhizosphere over the 41 d simulations. These simulations represent a root

system growing from seed at day 0, and remaining active in growth over the first 41 d. It was assumed that lecithin would play an important role for the majority of the young active root system over this time. Read et al. (2003) showed that lecithin has an effect on soil properties for a period of weeks in non-sterile soil, suggesting a low rate of degradation. Also, lecithin continued to affect soil properties in draining soil cores, suggesting a low mobility in the Bullionfield soil.

The initial simulations were designed to represent water and nutrient uptake at the rhizosphere-scale, with both models set up to replicate each other so that the two approaches could be compared. In both models, the rhizosphere soil had either the same water release and phosphate adsorption characteristics as the bulk soil, or these characteristics were altered by the presence of lecithin (Figure 1). The soil volume in the ROOTMAP model was $5 \times 5 \times 10$ mm, containing a 10 mm length of root. The 2D Finite Element Method model had a soil area of 5×5 mm, with the unit length results multiplied up for a 10 mm length of root. The ROOTMAP model had only two soil volumes, the bulk and rhizosphere volumes, and a time step of 600 s.

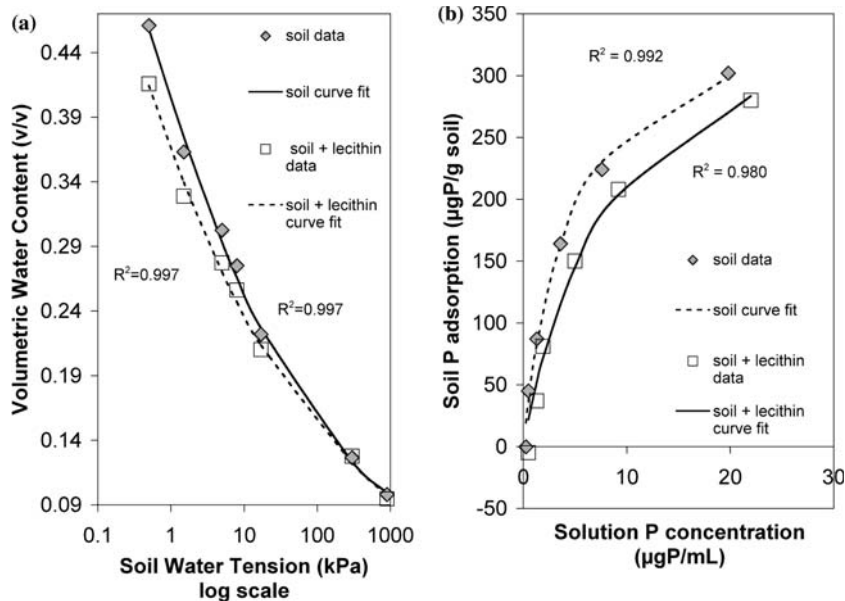


Figure 1. (a) Water release curves for Bullionfield Soil, with and without lecithin present. Symbols represent the experimental data from Read et al. (2003). Lines represent the fit of the van Genuchten (1980) soil water retention equation to the experimental data (Eqs. 1, 2). (b) Phosphate adsorption isotherms for Bullionfield soil, with and without lecithin present. Lines represent the fit of the Langmuir phosphate adsorption expression (Eq. 5) to the experimental data of Read et al. (2003).

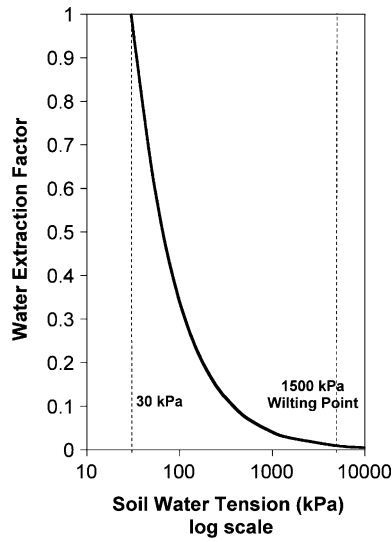


Figure 2. Water extraction factor $\alpha_w(\psi)$ (Eq. 7) included in the water uptake routine of the ROOTMAP model.

The Finite Element Method model utilised a grid structure comprised of approximately 1152 nodes, 2160 elements, and a time-step of 36 s. Total water, nitrate and phosphate over 12 h was calculated. This simulation period was chosen to correspond with the period of relatively high transpiration during the day. This 12 h simulation took 0.33 h to >2 h of CPU time (2 GHz Pentium PC) to run with the Finite Element Method model, and 5 s (Mac G4) with the ROOTMAP model.

In both models, the root radius was set to 0.2 mm, and soil density 1100 kg m^{-3} . Initial total available P was a uniform 177 mg/kg P , and initial nitrate 80 mg/kg N . Initial soil water potential varied from 30 kPa (0.201 v/v) to 200 kPa (0.135 v/v). Both models used Michaelis–Menten kinetics (parameters listed in Appendix).

ROOTMAP was used to investigate the interaction between lecithin exudation into the rhizosphere and nutrient acquisition by a growing and responsive root system. ROOTMAP was parameterised with architectural parameters representing wheat *Triticum aestivum* L. (with up to 6 seminal axes developing over time, and 1st to 3rd order laterals). To enable comparison with the rhizosphere-scale (10 mm root) simulations, all soil, water and nutrient parameters were left unchanged (uniform profiles). A second set of simu-

lations were run with half the initial N and P concentrations (88.5 mg/kg P , 40 mg/kg N , uniform initial profiles, concentrations decreasing over time resulting in a non-uniform final profile). Growth was simulated in a soil volume of $0.14 \times 0.14 \times 1 \text{ m}$, with no evaporation from the soil surface and no rainfall. The model was parameterised to represent a degree of plastic root growth response to nutrient supply typical of wheat plants (Robinson, 1994), and overall plant growth was affected by the level of soil resource supply. All results are the average of 4 simulations (replications). Since root growth is partially stochastically determined (Diggle, 1988), multiple runs with identical parameters produce non-identical root systems, and some variation in total water and nutrient uptake. Resource uptake was tracked for a simulated 41 d (~150 s CPU time, MacG4; starting from a wheat seed at time 0), with a time-step of 4 h.

Simulations were also run comparing water, nitrate and phosphate uptake of the wheat (*Triticum aestivum* L.) and a lupin (*Lupinus angustifolius* L.) root architecture. The lupin architecture was represented as a typical tap-rooted structure, dominated by the 1st order laterals, with some 2nd order branching (Dunbabin et al., 2002). All other parameters were identical for comparing between the two root architectures. For these root architecture comparisons, profiles of water, nitrate and phosphate availability decreasing with depth were used (Figure 3), simulating resource availability more typical of field soils.

Results

The aim of this work was to use lecithin exudation into the rhizosphere as a case study to investigate the value of scaling-up rhizosphere processes using plant models. Results are presented which compare water, nitrate and phosphate uptake predictions at the rhizosphere-scale by a detailed Finite Element Method model. The 3D root architecture model ROOTMAP, was then assessed for the ability to reproduce these predictions, and the interaction between lecithin exudation into the rhizosphere, and resource foraging by growing root architectures, was investigated.

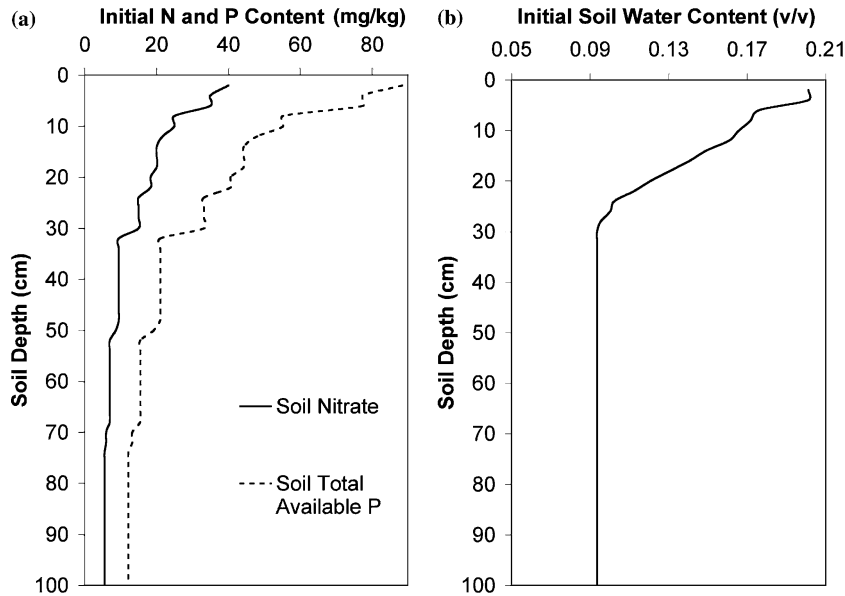


Figure 3. Soil nitrate (mg/kg N), total available P (mg/kg P) and water content (v/v) profiles used in simulations comparing resource acquisition by the contrasting lupin and wheat root architectures.

Water, nitrate and phosphate uptake by a 10 mm root segment over 12 h

The 2D Finite Element Method (FEM) model predictions for water, nitrate and phosphate uptake (over 12 h by 10 mm of root) are presented in Figure 4, and are a direct reflection of the effect of lecithin on the water release and phosphate adsorption characteristics of Bullionfield soil (Figure 1). Since lecithin reduces hydraulic conductivity at any given soil water potential (Read et al., 2003), water uptake was lower in the presence of lecithin, due to reduced transport across the rhizosphere. This effect was greatest at the wetter end of the scale, where water uptake over the 12 h was reduced by up to 16% (Figure 4a). Lecithin in the rhizosphere had little effect on nitrate uptake over the 12 h (Figure 4b). Since the initial nitrate concentration in these simulations was relatively high (80 mg/kg N, representing Bullionfield soil, Read et al. 2003), nitrate uptake was not transport limited over most of the moisture range, only falling at the drier end of the scale (Figure 4b). In contrast to this, phosphate uptake (Figure 4c) was transport limited over the entire moisture range. Lecithin reduces phosphate adsorption, increasing the proportion of phosphate in solution phase

(Figure 1b), hence P uptake was higher with lecithin present in the rhizosphere (Figure 4c). Since all simulations had the same initial total available P (177 mg/kg P), all were operating in the same region of the P adsorption isotherm (Figure 1b), with lecithin providing ~6% increase in P availability, resulting in a 3–4% increase in P uptake over the entire moisture range.

The 3D ROOTMAP model reproduced ($R^2 = 0.995\text{--}1.0$) the output of the 2D FEM model, for water, nitrate and phosphate uptake over the entire range of initial soil water potentials, and at all points over the 12 h time period (Figure 5).

Water, nitrate and phosphate uptake by a growing and responsive root system

The fundamental difference between the simulations of a whole root system and those of a 10 mm section of root, was the ability of the root system to grow and respond to the soil environment (initially uniform profiles become more heterogeneous through time due to local water and nutrient depletion). All results are presented as the ratio of resource uptake, or root growth, with lecithin present in the rhizosphere, relative to without. At the drier (relatively resource

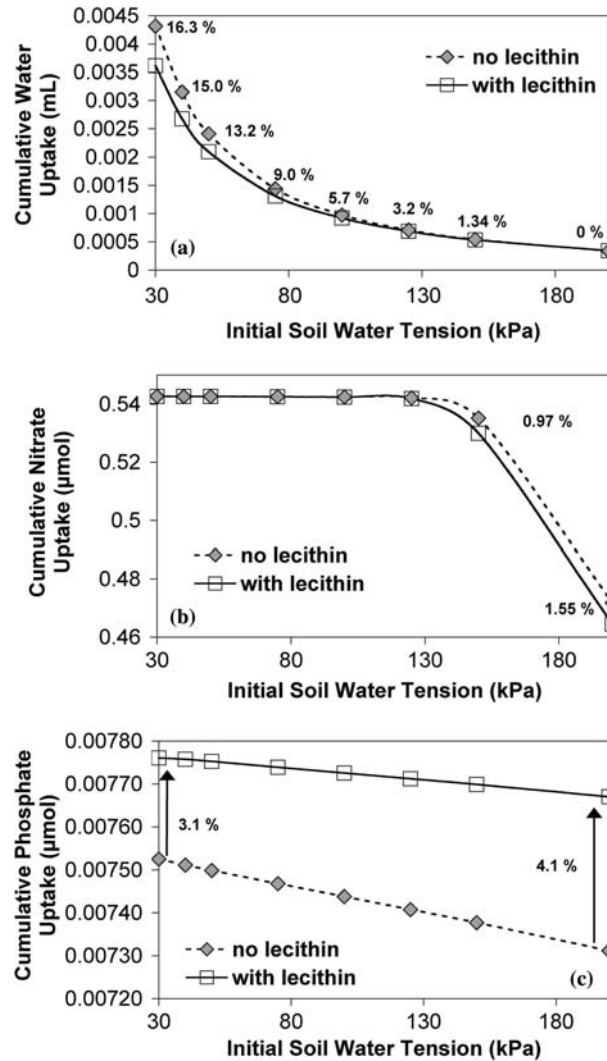


Figure 4. Cumulative resource uptake over 12 h by 10 mm section of root, with a range of initial soil water potentials, with or without lecithin present in the rhizosphere – output from the 2D Finite Element Method model. (a) Cumulative water uptake (mL). Percentage decrease in water uptake, due to lecithin being present in the rhizosphere is indicated on graph. (b) Cumulative nitrate uptake (μmol). Percentage decrease in nitrate uptake indicated on graph. (c) Cumulative phosphate uptake (μmol). Percentage increase in phosphate uptake indicated on figure.

limited) end of the scale, root surface area was 5–7% greater with lecithin exudation into the rhizosphere, than without (Figure 6b). The increase in P uptake (10–13%, 75–200 kPa; Figure 6b) was greater than that predicted from the rhizosphere-scale modelling (Figure 6a). On a per unit of root surface area basis, however, the P-benefit of lecithin exudation was similar to the 10 mm root case (Figure 6a, c). Lecithin had a decreasing effect on water acquisition in progressively drier soil, with the trend similar in the two scales

of modelling (Figure 6a, b). Since relative root growth increased in drier soil (Figure 6b), the decrease in water uptake was similar across the moisture range, when expressed on a per unit of root surface area basis (Figure 6c).

Relative nitrate uptake showed a very different trend in the whole root system modelling. Nitrate uptake was not transport limited over most of the moisture range for uptake by 10 mm of root over 12 h (Figures 4b, 6a). In contrast, nitrate depletion zones, and hence zones of relative

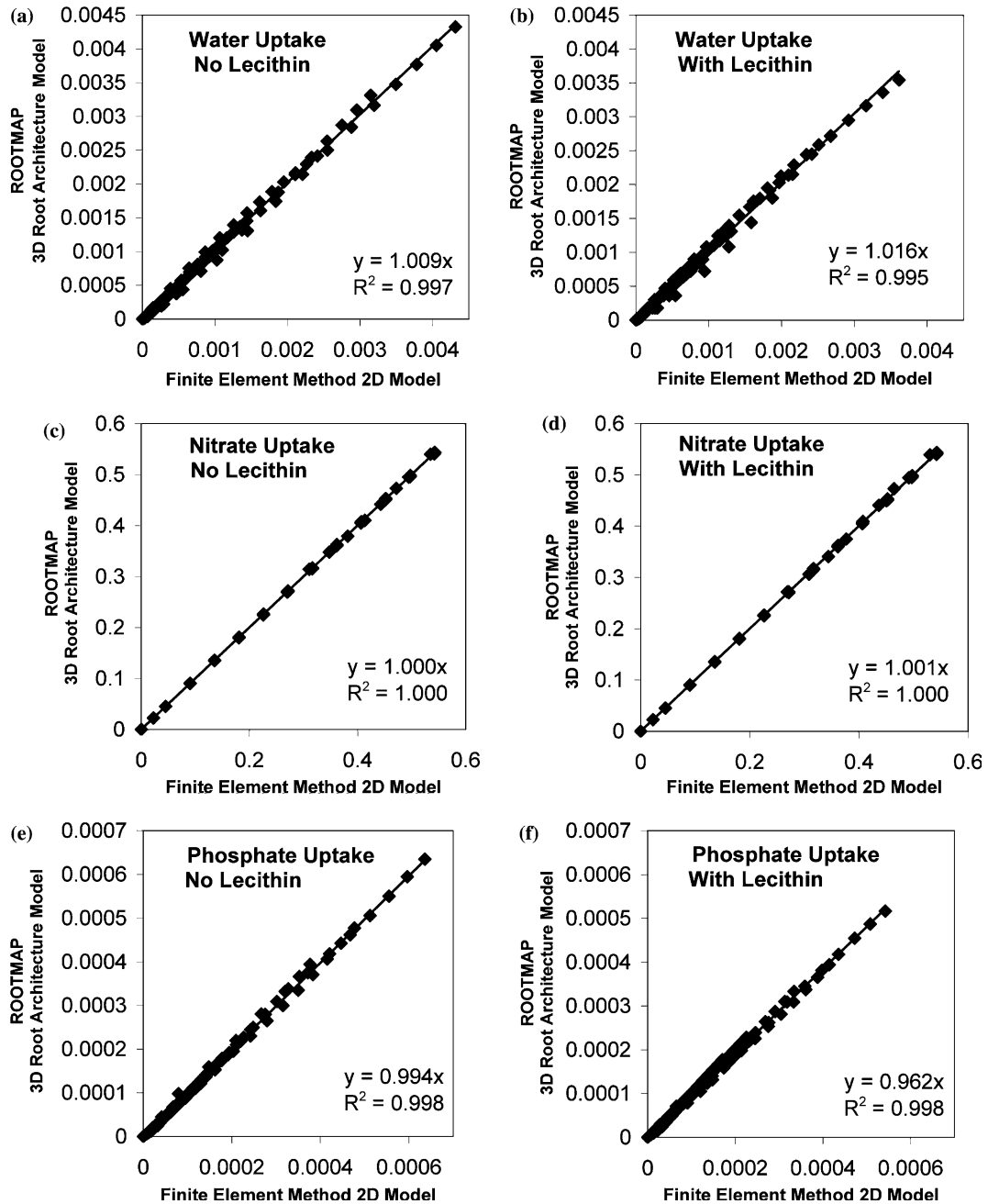


Figure 5. Comparison between the 2D Finite Element Method model and the 3D root architecture model ROOTMAP predictions of (a, b) water (mL), (c, d) nitrate (μmolN), and (e, f) phosphate (μmolP) uptake (for a 10 mm section of root). Data included are for the entire moisture range (30–200 kPa), and at intervals of 0.5 h over the 12 h simulations.

transport limitation, can develop around a whole root system (of complex root architecture) that is growing for 41 d. A reduction in both water and nitrate content in the rhizosphere leads to a decreased supply of N to the root surface by

both mass flow and diffusion. The effect of lecithin on nitrate (mobile resource) acquisition by the wheat root system followed the same trend as for water (mobile resource) uptake (Figure 6b, c).

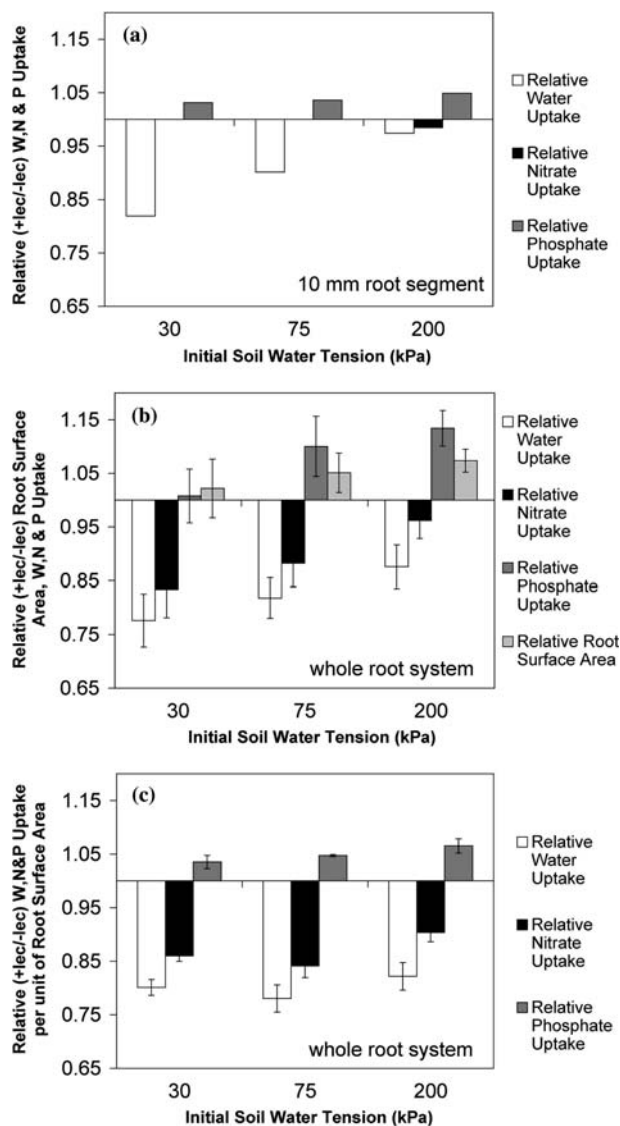


Figure 6. Water, nitrate and phosphate uptake and root surface area when lecithin is exuded into the rhizosphere relative to when there is no lecithin exudation. Relative uptake results from the (a) 10 mm root modelling; (b) the wheat (*Triticum aestivum* L.) root system modelling; and (c) the wheat root system modelling presented per unit of root surface area. The results for the wheat root system are the average of 4 model runs (replications). Initial N concentration 177 mg/kg N, initial P concentration 80 mg/kg. The vertical bars represent \pm s.e.

Simulations of resource acquisition from relatively nutrient poor soil (half the previous initial nutrient level; 88.5 mg/kg P, 40 mg/kg N), showed a different response characteristic to the results for relatively nutrient-rich soil. The benefit of lecithin exudation for phosphate acquisition was greater over the whole moisture range (Figure 7a). Even on a per unit of root surface area basis (Figure 7b), the benefit for P acquisition

was still 15 (75, 200 kPa) to 20% (30 kPa) greater in the lower nutrient soil (Figure 6c). There was a greater increase in root growth at the drier end of the scale (Figure 7a), and as a result, there was a smaller decrease in water and nitrate acquisition (Figures 7a, 6b). The water and nitrate uptake response was similar at both nutrient levels when expressed on a per unit of root surface area basis (Figures 6c, 7b).

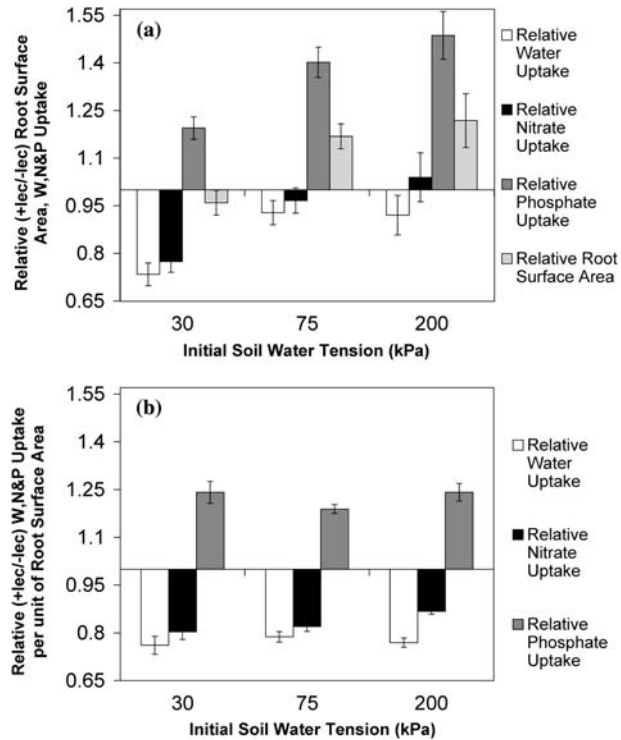


Figure 7. Water, nitrate and phosphate uptake and root surface area when lecithin is exuded into the rhizosphere relative to when there is no lecithin exudation, with half the initial nitrate and total available P content. Initial N concentration 88.5 mg/kg N, initial P concentration 40 mg/kg. Results from the (a) wheat (*Triticum aestivum* L.) root system modelling; and (b) the wheat root system modelling presented per unit of root surface area. The results are the average of 4 model runs (replications). The vertical bars represent \pm s.e.

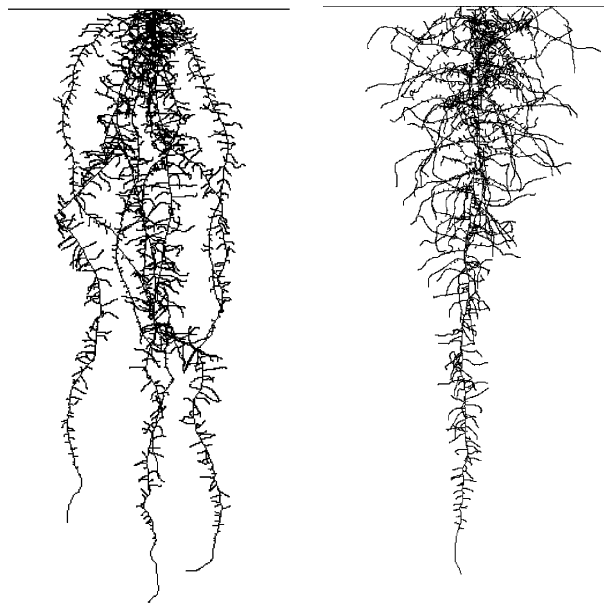


Figure 8. Example of the wheat (*Triticum aestivum* L.) and lupin (*Lupinus angustifolius* L.) root architectures used to investigate the effect of architectural form on water and nutrient acquisition by root systems exuding or not-exuding lecithin into the rhizosphere.

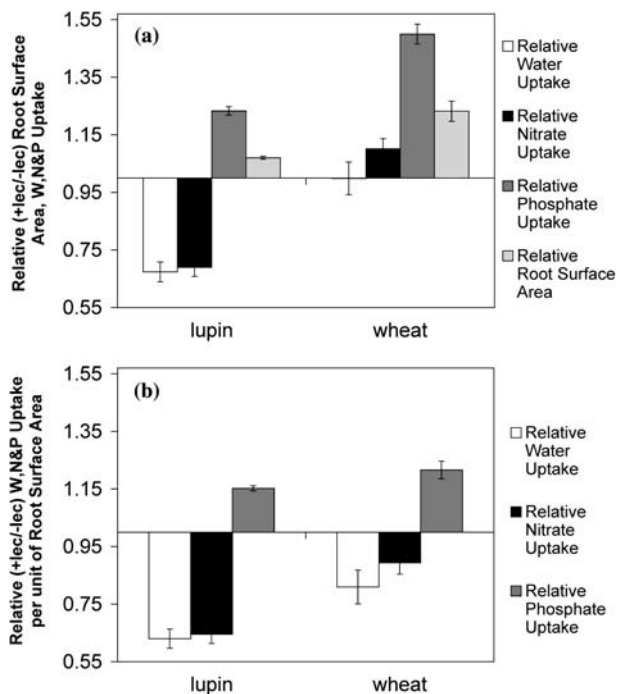


Figure 9. Comparison of root growth, and water, nitrate and phosphate uptake by wheat (*Triticum aestivum* L.) and lupin (*Lupinus angustifolius* L.) root systems. Results are for uptake with lecithin exudation relative to without. Results are presented on a per unit of root surface area basis in (b). The vertical bars represent \pm s.e.

Comparing nutrient acquisition by contrasting wheat and lupin root architectures

The results from simulations comparing wheat (*Triticum aestivum*) and lupin (*Lupinus angustifolius*) root architectures (Figure 8), suggest that root architectural form, and hence foraging potential, may influence the role that lecithin plays in nutrient acquisition from the rhizosphere. The simulation results show greater relative phosphate and nitrate acquisition, and greater relative root growth, for lecithin present in the wheat rhizosphere, than in the lupin rhizosphere (Figure 9). In these simulations, with nutrient and water availability declining with depth through the soil profile (Figure 3), the wheat response (Figure 9) was similar to that in the previous low water, low nutrient simulations (200 kPa, Figure 7). Water and nitrate uptake by the lupin root system was considerably reduced when lecithin was present in the rhizosphere (Figure 9).

Discussion

The results presented in this study highlight the value of investigating rhizosphere processes not only at the rhizosphere-scale, but also at the whole-plant scale. The degree to which lecithin exudation was predicted to be a cost or benefit to resource acquisition, changed between the scale of modelling, the level of resource supply, and the root architecture (Figures 6, 7, 9). Without the ability to represent growing, responsive root systems, rhizosphere-scale modelling is limited in its capacity to investigate the implications of rhizosphere processes on whole-plants.

The influence of lecithin on water and nutrient uptake at the rhizosphere-scale

Rhizosphere-scale modelling predicted a drop in water uptake of up to 16% (Figure 4a) in response to lecithin exudation, and an increase in phosphate uptake of a modest 3–4%, due to

decreased P adsorption. The challenge is to interpret these results in the context of a whole root system growing in a spatially and temporally variable environment. Growing and responsive root systems, rainfall frequency, seasonal variation in environmental factors, non-uniform nutrient distributions, fertiliser application, and potential interactions with bacterial populations and mycorrhizal fungi, all complicate the nutrient uptake environment, potentially overshadowing any 3–4% increase in phosphate availability and uptake.

It is important to note, however, that phosphorus is essentially a non-renewable resource, and of all the major nutrients, phosphorus is the least mobile, limiting crop production in most soils worldwide (Hinsinger, 2001). A 3–4% increase in availability may, therefore, represent an important increase in the potential for phosphate acquisition that could be exploited for improving the phosphate efficiency of crop varieties. P nutrition is such a valuable component of crop productivity that the capacity of lecithin to increase P availability to plants shows sufficient potential to justify further investigation.

The influence of lecithin on water and nutrient uptake at the root-system-scale

The close agreement between the 2D Finite Element Method (FEM) and 3D ROOTMAP models (Figure 5) provided the confidence that a whole root system model could reproduce the dynamics simulated by a more computationally expensive (FEM) rhizosphere model. ROOTMAP was then used to investigate some of the possible interactions between lecithin production and nutrient acquisition by growing and responsive root systems, over a longer time-scale.

Nitrate acquisition showed a different trend in the root system modelling, compared to that predicted from the rhizosphere-scale modelling. While nitrate uptake was not transport limited in the simulations of uptake by 10 mm of root over 12 h (Figures 4b, 6a), there was a substantial reduction in the rhizosphere nitrate and water content of the root system growing over 41 d. This limited nitrate transport to the root surface by mass flow and diffusion. The presence of lecithin further reduced water transport to the rhizo-

sphere (lower hydraulic conductivity), resulting in a decrease in water uptake of up to 20%. Nitrate uptake, in turn, decreased by up to 15% (30 kPa, Figure 6b), due to decreased nitrate transport by mass flow and diffusion. Also, lower resource uptake meant less root growth. This had a small effect on resource uptake early in the simulation, when water and nutrient contents were still high. The greatest impact came later in the 41-d period when there was a substantial reduction soil resources. A reduced growth rate meant a reduced capacity to explore and access new, un-depleted soil volumes, restricting the root system to already depleted zones.

The decrease in nitrate uptake may be exacerbated further when considering the contribution of N mineralisation to N uptake. Read et al. (2003) found that lecithin reduced the rate of N mineralisation in Bullionfield soil. In soils where N mineralisation provides all, or a large proportion of the plant available N, any reduction in the rate of N mineralisation may have a significant effect on N acquisition. This may be particularly true in topsoil layers where organic N contents are highest, and root length density, and the proportion of rhizosphere soil, is also highest.

In addition to the work of Read et al. (2003), other investigations have shown that root mucilage may reduce water content and water transport in rhizosphere soil. Whalley et al. (2004) found that the infiltration of water into the rhizosphere of maize was significantly lower than into bulk soil, with a corresponding reduction in hydraulic conductivity. Whalley et al. (2004) hypothesised that the higher density of the rhizosphere soil (caused by the displacement of soil particles as roots elongate) may explain the lower hydraulic conductivity in the rhizosphere compared to bulk soil.

Czarnes et al. (2000) found that polygalacturonic acid (PGA; used as a root mucilage analogue), reduces water sorptivity and increases water repellency on soil surfaces, resulting in a slower rate of water infiltration into rhizosphere soil. While the immediate implication of this is reduced water availability, Czarnes et al. (2000) suggested that PGA (root mucilage) may stabilise soil aggregates in the rhizosphere, increasing soil strength and dampening the wetting and drying cycles that can crack and destabilise rhizosphere soil.

It is clear from these examples that water dynamics in the rhizosphere are complex, and may be influenced by a range of factors. While rhizosphere soil density and the chemical content of root mucilage may act to reduce water infiltration into rhizosphere soil, mucilage may help to stabilise rhizosphere soil aggregates, improving root-soil contact. Further research is needed to develop a better understanding of the costs and benefits of root mucilage to water and nutrient acquisition at the rhizosphere and plant scales.

From the ROOTMAP simulations, the benefit of lecithin for P acquisition was 8% greater for a growing root system, than a static, 10 mm section of root (Figure 6a, b). This was due largely to an increase in root growth, with uptake per unit of surface area similar between the two scales of modelling (Figure 6a, c). The modelled plant (with phosphate-limited growth) utilised the additional phosphate taken up (with lecithin present) to produce additional internal assimilate for future growth. This feedback system led to a larger plant with a larger root system for further P foraging. The benefit was greatest in the driest soil (200 kPa; Figure 6b), suggesting that plants growing in relatively resource-poor soil may gain the greatest benefit from increased P availability in the rhizosphere. Low resource supply places a limit on plant and root growth. Increased growth due to an increase in P availability can enable the root system to explore new, un-depleted soil volumes, further increasing access to P. The simulations with half the initial nitrate and phosphate content support this, with the benefit of lecithin for P acquisition 10–27% greater than in the high-nutrient case.

The work of Liebersbach et al. (2004) also suggests that plants may receive the greatest benefit from compounds in root mucilage when soil is dry. Mucilage from water-stressed plants increased P concentration in soil solution under dry conditions, which intern increased P uptake by oat and sugar beet in dry soil (Liebersbach et al., 2004). The rate of mucilage exudation by oat and maize has been found to increase in dry soil (Czarnes et al., 2000; Liebersbach et al., 2004), further suggesting that the exudation of mucilage may be a mechanism for improving nutrient availability when soil water content is low.

Since the FEM model took anywhere from 0.33 h to >2 h to simulate uptake over 12 h (see

Model Parameterisation section), there was a limit in the ability to represent agriculturally important time-scales. The ROOTMAP model, on the other hand, represented a potentially lower degree of detail and accuracy, using a coarser grid and larger time-step. ROOTMAP did, however, reproduce the FEM model results well (Figure 5) and could run the same simulation in a fraction of the time (5 s), and easily represent time-scales of months (41 d taking around 150 s to run in these simulations). This ability to simulate root systems growing over months and seasons is important for scaling-up rhizosphere processes, and investigating their impact on plant and crop growth over a growing season.

The interaction between root architecture and resource acquisition, with and without lecithin exudation

Phospholipid surfactants have been found in maize, lupin and wheat root mucilage (Read et al., 2003). While the relative effect of these lipids on resource acquisition by the three species is not known, differences in root architecture, and hence resource foraging capacity, may be important. This is an area where root architectural models can play a role in scaling-up and investigating interactions between rhizosphere processes and root foraging potential.

Simulations of the contrasting wheat (*Triticum aestivum* L.) and lupin (*Lupinus angustifolius* L.) root architectures (Figures 8, 9), suggested that a wheat root architecture may gain a greater benefit from lecithin exudation into the rhizosphere, than a lupin root architecture. Previous theoretical studies have certainly shown that root architecture can play an important role in the efficiency with which mobile and immobile nutrients are acquired from soil.

Studies by Fitter and colleagues (Fitter, 1985, 1987; Fitter et al., 1991) have suggested that highly branched root architectures are more efficient at the capture of immobile ions, such as phosphate, than more sparsely branched root systems. In addition to this, Lynch and Brown (2001) demonstrated, through modelling and plant experiments, a link between the capacity for topsoil foraging and the phosphate acquisition efficiency of bean cultivars. These findings support the results of this study, which suggest that due to the foraging strategy, a highly

branched wheat root system may take greater advantage of increased phosphate availability (with lecithin), than a lupin root system.

The wheat root system (Figure 8) had multiple root axes, maximising the total volume of soil explored, and up to 3 orders of branching, maximising intensity of resource exploration, particularly in the relatively nutrient-rich topsoil layers (Figure 3). In contrast, the lupin root architecture consisted of only the single main axis, first order branches, and limited second order branching. This root architecture had limited potential to plastically respond to the non-uniform resource supply, and was particularly limited in the capacity to allocate roots to, and hence forage in, the resource-rich topsoil layers. The benefit of lecithin exudation for P acquisition by lupin-type root architectures cannot, however, be discounted. The lupin root architecture did still obtain a P benefit from lecithin exudation into the rhizosphere, and while less nitrate was acquired (Figure 9), this will have a reduced effect on N₂-fixing plants.

Conclusion

Much of the value of modelling lies in the ability to represent and investigate complex and inaccessible systems. To quantify experimentally the effect that phospholipid surfactants, present in root mucilage, have on water and nutrient acquisition by plants, a mutant not producing these lipids would be required for comparison with lipid-producing plants. In the absence of such a mutant, the modelling exercise undertaken in this study provides the important first-step in investigating some of the interactions between lecithin exudation and resource acquisition. In particular, this study highlights the value of including rhizosphere processes into plant and crop models for investigating the effect of responsive root growth and root architecture, and agriculturally relevant time-scales, on resource acquisition in plant systems.

Appendix 1

$$\theta = \frac{\theta_s - \theta_r}{[1 + (\alpha\psi)^{n/m}] + \theta_r} \quad m = 1 - 1/n \quad (1)$$

$$\begin{aligned} K &= K_S \Theta^{1/2} [1 - (1 - \Theta^{1/m})^m]^2 \\ &= K_S \frac{[1 - (\alpha\psi)^{n-1} [1 + (\alpha\psi)^n]^{-m}]^2}{[1 + (\alpha\psi)^n]^{m/2}} \end{aligned} \quad (2)$$

Θ = normalised volumetric water content; θ = volumetric water content; θ_s , θ_r = saturated and residual volumetric water contents; α , n = fitting parameters; Ψ = soil water potential; K = unsaturated hydraulic conductivity; K_s = saturated hydraulic conductivity. $n(\text{lecithin}) = 1.1932$; $n(\text{no lecithin}) = 1.2121$; $\alpha(\text{lecithin}) = 1.1566$; $\alpha(\text{no lecithin}) = 0.5428$; $\theta_s = 0.5926$; $K_s = 0.0026$.

$$I = I_{\max} \frac{c - c_{\min}}{K_m + (c - c_{\min})} \quad (3)$$

I = influx of solute; c = concentration of solute; c_{\min} = solute concentration at zero net influx; K_m = kinetic constant. $I_{\max} = 15 \text{ nmol m}^{-2} \text{ s}^{-1}$, $K_m = 10 \text{ mmol m}^{-3}$, $C_{\min} = 0.1 \text{ mmol m}^{-3}$, for phosphate uptake. $I_{\max} = 1.0 \text{ } \mu\text{mol m}^{-2} \text{ s}^{-1}$, $K_m = 10 \text{ mmol m}^{-3}$, $C_{\min} = 0.1 \text{ mmol m}^{-3}$, for nitrate uptake (pers. comm. D. Robinson).

$$Q = \frac{\psi_s - \psi_l - \Delta P}{R} \quad (4)$$

Q = transpiration rate; Ψ_s = soil water potential at the root surface; Ψ_l = leaf water potential; R = hydraulic resistance of the plant. ΔP = minimum pressure difference required for water flow in the plant. $\Psi_l = -0.5 \text{ MPa}$ constant.

$$x = \frac{QbC}{1 + bC} \quad (5)$$

x = solute adsorbed solid phase P; C = solute concentration of liquid phase P; Q = maximum adsorption capacity; b = affinity coefficient. $Q(\text{lecithin}) = 11.863$; $Q(\text{no lecithin}) = 12.745$; $b(\text{lecithin}) = 6.828$; $b(\text{no lecithin}) = 3.584$.

$$\begin{aligned} \frac{d\bar{C}_{li}}{dt} &= \frac{-2\pi a_i \alpha_i L_i}{b} \\ &\times \frac{\bar{C}_{li}}{\frac{\alpha_i}{w_i} + \left(1 - \frac{\alpha_i}{w_i}\right) \left(\frac{2}{2 - \frac{\alpha_i w_i}{Db}}\right) \left(\frac{\left(\frac{x}{a_i}\right)^{2 - (\alpha_i w_i / Db)} - 1}{\left(\frac{x}{a_i}\right)^2 - 1}\right)} \end{aligned} \quad (6)$$

$$S_w = T_{\max} \alpha_w(\psi) L(x, y, z) \quad (7)$$

S_w = water uptake rate; T_{\max} = maximum transpiration rate; ψ = soil water potential in the rhizosphere; $L(x, y, z)$ root length density in 3D space.

$$q = -K\nabla\psi \quad (8)$$

q = water flux; K = unsaturated hydraulic conductivity; ψ = soil water potential.

Acknowledgements

The authors would like to thank Dr K. Zhang for coding much of the 2D Finite Element Method model. Profs P. Gregory, D. Robinson, I. Young, J. Crawford and Dr D. Read are thanked for helpful discussions. This study was supported by the Grains Research and Development Corporation, through a fellowship held by the senior author, and by funds from the Biotechnology and Biological Sciences Research Council. The Scottish Crop Research Institute Receives Grant-In-Aid from the Scottish Executive Environment and Rural Affairs Department.

References

- Arah J 2001 Incorporating rhizosphere processes into field-scale (agro)ecosystem models. *Plant Soil*. 232, 119–127.
- Baldwin J P, Nye P H and Tinker P B 1973 Uptake of solutes by multiple root systems from soil. III. A model for calculating the solute uptake by a randomly dispersed root system developing in a finite volume of soil. *Plant Soil*. 38, 621–635.
- Bowen G D and Rovira A D 1999 The rhizosphere and its management to improve plant growth. *Adv. Agron.* 66, 1–102.
- Calba H, Cazevielle P and Jaillard B 1999 Modelling of the dynamics of Al and protons in the rhizosphere of maize cultivated in acid substrate. *Plant Soil*. 209, 57–69.
- Clarkson D T and Lüttge U 1991 Inducible and repressible nutrient transport systems. *Prog. Bot.* 52, 61–83.
- Czarnes S, Hallett P D, Bengough A G and Young I M 2000 Root- and microbial-derived mucilages affect soil structure and water transport. *Eur. J. Soil Sci.* 51, 435–443.
- Darrah P R 1996 Rhizodeposition under ambient and elevated CO₂ levels. *Plant Soil*. 187, 265–275.
- Darrah P and Roose T 2001. Modeling the rhizosphere. *In The Rhizosphere: Biochemistry and Organic Substances at the Soil-Plant Interface.* pp 327–372. Marcel Dekker Inc. New York.
- Diggle A J 1988 ROOTMAP – a model in three-dimensional coordinates of the growth and structure of fibrous root systems. *Plant Soil*. 105, 169–178.
- Dunbabin V M, Diggle A J, Rengel Z and Hugten Rvan 2002 Modelling the interactions between water and nutrient uptake and root growth. *Plant Soil*. 239, 19–38.
- Feddes R A, Kowalik P, Kolinska-Mayinka K and Zaradny H 1976 Simulation of field water uptake by plants using a soil water dependent root extraction function. *Hydrology* 31, 13–26.
- Fitter A H 1985. Functional Significance of Root Morphology and Root System Architecture. *In Ecological Interactions in Soil.* pp 87–106. Blackwell Scientific Publications, Oxford.
- Fitter A H 1987 An architectural approach to the comparative ecology of plant root systems. *New Phytol.* 106, 61–71.
- Fitter A H, Stickland T R, Harvey M L and Wilson G W 1991 Architectural analysis of plant root systems. 1. Architectural correlates of exploitation efficiency. *New Phytol.* 118, 383–389.
- Gahoonia T S and Nielsen N E 2004 Root traits for creating phosphorus efficient crop varieties. *Plant Soil*. 260, 47–57.
- Hinsinger P 2001 Bioavailability of soil inorganic P in the rhizosphere as affected by root-induced chemical changes: a review. *Plant Soil*. 237, 173–195.
- Huang K, Mohanty B P, Leij F J and Genuchten Th Mvan 1998 Solution of the nonlinear transport equation using modified Picard iteration. *Adv. Water Resour.* 21, 237–249.
- Jones D L, Darrah P R and Kochian L V 1996 Critical evaluation of organic acid mediated iron dissolution in the rhizosphere and its potential role in root iron uptake. *Plant Soil*. 180, 57–66.
- King B J, Siddiqi M Y, Ruth T J, Warner R L and Glass A D M 1993 Feedback regulation of nitrate influx in barley roots by nitrate, nitrite and ammonium. *Plant Physiol.* 102, 1279–1286.
- Kirk G J D 2001 Plant-mediated processes to acquire nutrients: nitrogen uptake by rice plants. *Plant Soil*. 232, 129–134.
- Kirk G J D 2002a Use of modelling to understand nutrient acquisition by plants. *Plant Soil*. 247, 123–130.
- Kirk G J D 2002b Modelling root-induced solubilization of nutrients. *Plant Soil*. 255, 49–57.
- Liebersbach H, Steingrobe B and Claassen N 2004 Roots regulate ion transport in the rhizosphere to counteract reduced mobility in dry soil. *Plant Soil*. 260, 79–88.
- Lynch J P and Brown K M 2001 Topsoil foraging - an architectural adaptation of plants to low phosphorus availability. *Plant Soil*. 237, 225–237.
- McCully M E 1999 Roots in soil: Unearthing the complexities of roots and their rhizospheres. *Annu. Rev. Plant.* 50, 695–718.
- Neumann G and Römheld V 2002. Root induced changes in availability of nutrients in the rhizosphere. *In Plant Roots: The Hidden Half.* Eds. Y Waisel, A Eshel and U Kafkafi. pp 617–649. Marcel Dekker, New York.
- Read D B, Bengough A G, Gregory P J and 6 others 2003 Plant roots release phospholipid surfactants that modify the physical and chemical properties of soil. *New Phytol.* 157, 315–326.
- Robinson D 1994 The responses of plants to non-uniform supplies of nutrients. *New Phytol.* 127, 635–674.
- Roose T and Fowler A C 2004 A mathematical model for water and nutrient uptake by plant root systems. *J. Theoret. Biol.* 228, 173–184.
- Toal M E, Yeomans C, Killham K and Meharg A 2000 A review of rhizosphere carbon flow modelling. *Plant Soil*. 222, 263–281.

- van Genuchten, M 1980 A closed-form equation for predicting hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* 44, 892–898.
- Whalley W R, Leeds-Harrison P B, Leech P K, Riseley B and Bird N R A 2004 The hydraulic properties of soil at root-soil interface. *Soil Sci.* 169, 90–99.
- Zhang H and Forde B G 1998 An Arabidopsis MADS box gene that controls nutrient-induced changes in root architecture. *Science* 279, 407–409.