Mathematical models of plant–soil interaction

BY TIINA ROOSE 1,* AND ANDREA SCHNEPF 2

1 OCIAM and CMB, Mathematical Institute, University of Oxford, 24–29 St Giles, Oxford OX1 3LB, UK
2 Institute of Soil Science, Department of Forest and Soil Sciences, BOKU–University of Natural Resources and Applied Life Sciences, Peter Jordan-Strasse 82, 1190 Vienna, Austria

In this paper, we set out to illustrate and discuss how mathematical modelling could and should be applied to aid our understanding of plants and, in particular, plant–soil interactions. Our aim is to persuade members of both the biological and mathematical communities of the need to collaborate in developing quantitative mechanistic models. We believe that such models will lead to a more profound understanding of the fundamental science of plants and may help us with managing real-world problems such as food shortages and global warming. We start the paper by reviewing mathematical models that have been developed to describe nutrient and water uptake by a single root. We discuss briefly the mathematical techniques involved in analysing these models and present some of the analytical results of these models. Then, we describe how the information gained from the single-root scale models can be translated to root system and field scales. We discuss the advantages and disadvantages of different mathematical approaches and make a case that mechanistic rather than phenomenological models will in the end be more trustworthy. We also discuss the need for a considerable amount of effort on the fundamental mathematics of upscaling and homogenization methods specialized for branched networks such as roots. Finally, we discuss different future avenues of research and how we believe these should be approached so that in the long term it will be possible to develop a valid, quantitative whole-plant model.

Keywords: multiscale modelling; soil–plant–atmosphere continuum; climate change

1. Introduction

Plant and soil processes and their interactions are an important part of the soil–plant–atmosphere continuum, affecting issues such as climate change and carbon cycling, as well as rhizotechnologies, agriculture and bioremediation. Within the plant–soil–atmosphere continuum, atmosphere and climate have received much attention in comparison with the below-ground processes that inevitably would include plant and soil interactions (Feddes et al. 2001; Wang & Smith 2004). This is due to the fact that the below-ground processes, particularly the dynamic

* Author for correspondence (roose@maths.ox.ac.uk).


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ones, are difficult to assess with experiments (Toal et al. 2000; Feddes et al. 2001). However, mechanistic understanding of the plant–soil interaction is clearly needed if we are to be able to continue providing affordable food for an ever-increasing human population. In March 2008, the BBC reported that the price of spring wheat had doubled in two months (news.bbc.co.uk) owing to droughts in China and Australia. Thus, even in the short term, it is necessary to know how climate change can influence crop yields. Mathematical modelling of the plant–soil interaction can undoubtedly play a role in predicting such events (see references in the electronic supplementary material).

A distinct feature of the soil–plant–atmosphere continuum is that the phenomena occur on several spatial and temporal scales and the feedback loops between these scales can become significant when assessing their overall impact on crop growth and climate change (figure 1). Models on the single-root scale have given insight into the complex dynamic phenomena that occur around the root. This region in the soil around a root has been loosely named as ‘rhizosphere’ (Hiltner 1904; Tinker & Nye 2000; Darrah et al. 2006) and models dealing with this are called rhizosphere models.

The term ‘rhizosphere’ was first coined by Hiltner (1904), and it referred to the region of soil immediately surrounding the root that is influenced by root activities. While at first glance this might be a relatively well-defined region, on closer observation it is not, since even small changes in the soil near the root could lead to global changes in the soil properties on the whole-plant scale. Mathematical models...
on the scale of a whole-plant root system deal with assessing the impact of rhizosphere phenomena at the plant scale. In addition, these models enable the assessment of the roles that feedback loops between nutrient acquisition and plant growth can have on overall crop growth and development.

We are convinced that rigorous mathematical methods offer an important tool for enhancing our understanding and ability to adequately manage the plant–soil continuum. In this paper, we describe the methods used to model the plant–soil interaction and how this technology should be developed further to make a true impact on science. Thus, this paper is not a review paper and it is not intending to give a comprehensive literature review of all the processes and feedback loops inherent in the plant–soil continuum. Instead, we aim to describe the general flavour of the modelling techniques and methodologies that would, in our opinion, enrich the scientific understanding more profoundly.

We describe the most commonly used mechanistic mathematical models for nutrient and water uptake by plants. We focus on their strengths and weaknesses, and we also discuss what type of mathematical methodology needs to be developed in order to make rigorous progress in incorporating these models into climate change and crop growth models. There is a wealth of serious mathematical literature on modelling of fluid flow in porous media (e.g. Hornung 1997; Panfilov 2000) applied to understanding the movement of water, pollutants, etc. in the soil. However, this technology has not been translated as effectively as it could have been into the plant–soil interaction area owing to it being unapproachable to non-specialist/non-mathematical audiences. This is largely because a significant number of these homogenization and upscaling technologies are presented in very pure mathematical journals and researchers working in this area appear not to be interested in the immediate, practical applicability of their results to specific experimental situations. We expect this to be remedied in the next couple of years by closer collaboration between experimentalists and mathematical modellers. In the plant and soil science community, this is currently known as ‘upscaling’, e.g. from the single-root scale to root system and field scale, and has for some time been recognized as a challenge (Darrah et al. 2006; Raats 2007). This is because the phenomena on a single-root scale are complex and dynamic, leading necessarily to models that have so far only been solved numerically. While the dynamics of isolated aspects of the rhizosphere can be well characterized experimentally, their cumulative effect and the proportion of the individual processes responsible for that cumulative effect cannot very easily be assessed experimentally without the input from mathematical modelling. Roose & Fowler (2004a) have shown that different mathematical techniques for upscaling nutrient uptake can theoretically lead to 30 per cent differences between computed uptakes. It is therefore necessary that suitable upscaling and homogenization techniques are used and developed further to make models mathematically rigorous and scientifically useful. Otherwise, wrong conclusions about the system behaviour could be drawn.

2. Multiscale models of the plant–soil interaction

All single-root scale rhizosphere models have grown out of the pioneering work done in 1960 by the groups led by Peter Nye in Oxford and Stanley Barber in Purdue (Olsen & Kemper 1968; Barber 1995; Tinker & Nye 2000). Since then,
they have been used to study nutrient uptake, contaminant (zinc, cadmium, lead, etc.) uptake by a single root, microbial dynamics in the vicinity of a single root and the effect of organic ligands exuded by the root into the soil on the bioavailability of phosphate (see references in the electronic supplementary material). Most of these models consider water saturation in the soil to be constant. However, some of the recent models have incorporated water flow inside the root and in the soil (Roose & Fowler 2004a; Doussan et al. 2006). In this section, we describe some of the most common models that have been applied to single-root and root-system plant–soil interaction, and, further on, discuss the models that consider additional effects, such as root hairs, soil fungi and microbes.

(a) Root nutrient uptake

In this section, we discuss the models for nutrient uptake by a single cylindrical root. In the following, we present water uptake models. All single-root scale models of nutrient uptake consider mass balances of solutes (nutrients, pollutants, etc.), with concentration \( c \) in the fluid phase and the amount \( c_s \) bound to the solid particles. In general, two assumptions are made: (i) the solute binding and debinding to and from the solid particles is in fast equilibrium compared with the transport time scale, and (ii) the transport in the fluid phase is given by diffusion and convection, and solutes bound to the soil particles are immobile. This results in the following transport equation for the solutes \( c \) in the fluid phase (Tinker & Nye 2000):

\[
\partial_t [(b + \theta)c] + \nabla \cdot (vc) = \nabla \cdot (Df\theta\nabla c),
\]  

(2.1)

where \( b \) is the soil buffer power, and hence \( c_s = bc \) is the total amount of solute bound to the soil particles; \( \theta \) is the volumetric soil water content, and thus \( c_s + \theta c = (b + \theta)c \) is the overall amount of solute per unit volume of soil; \( D \) is the solute diffusivity in water; \( f \) is the soil impedance factor, and therefore \( Df\theta \) is the effective diffusion coefficient for the solute in the soil; and \( v \) is the water flux in the soil. If we know the flux of fluid \( V \) into the single cylindrical root, we find that \( v = v(r) = -aV/r \), where \( a \) is the root radius and \( V \) is the water flux into the root. The plant–soil interaction is included in this model via a boundary condition that describes the rate of nutrient flux into the root, i.e.

\[
Df\theta n c - c(n \cdot v) = \frac{V_{\text{max}} c}{K_m + c} - \frac{V_{\text{max}} c_{\text{min}}}{K_m + c_{\text{min}}} \text{ at } r = a,
\]  

(2.2)

where \( \theta n \) is the derivative normal to the root surface with unit normal vector \( n \); \( V_{\text{max}} \) is the maximum solute influx into the root; \( K_m \) is the concentration of the solute when the flux of it into the root is half of maximum; and \( c_{\text{min}} \) is the level of the solute when the uptake by roots stops. Far away from the root, the majority of models assume that either the concentration is undisturbed by the root \( (c \to c_0 \text{ as } r \to \infty) \) or the presence of another root at distance \( r = d/2 \) gives rise to a reflection boundary condition \( (Df\theta n c - c(n \cdot v) = 0 \text{ at } r = d/2) \).

While equation (2.1) itself is linear when \( b \) and \( \theta \) are constant, due to the nonlinearity in the boundary condition (2.2), analytical solutions of the model cannot be found explicitly. This has made the upscaling of modelling from the
single-root scale to the root-system scale difficult. However, some progress in understanding this model can be made if one uses a combination of dimensionless analysis and the method of matched asymptotic expansion.

Dimensionless analysis identifies the importance of different processes included in the model in comparison with one another. For example, in equation (2.1), there is only one dimensionless grouping of parameters that makes a quantitative difference to the solutions. This grouping is called the Péclet number and it is obtained by balancing the diffusion and time-derivative terms with the convection term, i.e. the Péclet number is given by \( Pe = a V / (Df) \). It has been found in Roose et al. (2001) and Roose & Kirk (in press) that the convection of most nutrients and pollutants that plants take up is negligible (i.e. the convection term in equation (2.1) can be ignored). However, in cases when the nutrient uptake is very small, i.e. when the convective flux \( Vc \) is of the same order as the rate of uptake \( V_{\text{max}} c / (K_m + c) \), then the convection term (which is linear) should be retained in the boundary condition (2.2), but it can be safely neglected in (2.1). Next, we can use asymptotic analysis tools to find analytical expressions for the solute flux into the cylindrical root. This asymptotic analysis is based on the following considerations: (i) finding a solution that is valid far away from the root surface, (ii) finding a separate solution that is valid near the root surface, and then (iii) matching the two solutions together in the intermediate region where both solutions are valid. Using this technique, Roose et al. (2001) have found that the analytical solution to the flux of solute into the root is given by

\[
F(t) = V_{\text{max}} \frac{2c_\infty}{1 + c_\infty + L(t) + \sqrt{4c_\infty + (1 - c_\infty + L(t))^2}}, \tag{2.3}
\]

where \( c_\infty = c_0 / K_m \); \( \lambda = V_{\text{max}} a / (Df K_m) \);

\[
L(t) = \frac{\lambda}{2} \ln \left( 4 e^{-\gamma} \frac{Df \theta t}{(b + \theta) a^2} + 1 \right);
\]

and \( \gamma \) is Euler’s constant. The ability to derive this analytical expression for the flux of nutrient into a single cylindrical root not only serves as an enormous help when fitting experimental data on single-root scale measurements, but also, more importantly, makes the upscaling from the single-root scale model to the root-system scale model much simpler.

In this section, we described a model for the uptake of a single solute by the plant. However, it is clear that more complex speciation of nutrients could be included in the model together with competitive uptake. However, owing to complex soil chemical speciation and difficulties in parametrizing competitive uptake, this type of model is rarely performed.

(b) Root water uptake

In addition to mineral nutrients, plants also need water for their growth and function. In this section, we describe models that deal with water uptake by a single root. The early modelling work in this area was carried out by Philip (1966), Dalton et al. (1975) and Herkelrath et al. (1977a,b) in the 1960s and 1970s, and we recommend interested researchers to read these four review papers that highlight the importance of modelling and its pitfalls. There are three types of models for water flow on the single-root scale. The first type deals with water flow inside the...
root and considers simplified water flow within the soil. The second type deals with water flow in the soil and does not take account of water flow within roots (for further information on both approaches, see Molz (1981), Passioura (1988), Hopmans & Bristow (2002) and Raats (2007)). The third type combines both approaches and deals with water flow both inside the roots and in the soil (Roose & Fowler 2004a; Doussan et al. 2006). While Roose & Fowler (2004a) consider multiscale analysis and derive a fully coupled field-scale model useful for inclusion in climate and agricultural management models, Doussan et al. (2006) incorporated a detailed three-dimensional root structure and temporal evolution of root water uptake characteristics that can be used to answer specific questions about the root architecture in the water uptake limiting situations.

The essential ingredient of any water uptake model is the description of the internal root water pressure or potential distribution, where the conversion between the two is simple enough. The water balance within roots can be calculated by balancing the flux along the root, the so-called axial flux, \( q_z \), with the flux of water into the root, the so-called radial flux \( q_r \). Water flows axially from roots to leaves along the xylem vessels, and this flow is well characterized by a sum of Poiseuille flows over all sizes of the xylem vessels, i.e.

\[
q_z = -k \left( \frac{\partial p_r}{\partial z} - \rho g \right), \quad k = \sum_i \frac{\pi n_i R_i^4}{8\mu},
\]

where \( n_i \) and \( R_i \) are the number and radius of different size class \( i \) functional xylem vessels; \( \mu \) is the viscosity of water; \( p_r \) is the water pressure inside the root; and \( \rho g \) represents the gravitational potential gradient.

The leading-order radial movement of water from the soil to the xylem vessels can be taken to be proportional to the difference in the fluid pressure (or potential), i.e.

\[
q_r = k_r (p - p_r),
\]

where \( k_r \) is the axial conductivity of the root cortex to water and \( p \) is the fluid pore pressure in the soil at the root surface. Crucially, \( p \) depends on the soil saturation \( S \) via the soil–water retention curve (Van Genuchten 1980), i.e. \( p = p(S) \). Thus, the mass balance for water in the single root is given by

\[
2\pi a k_r [p(S) - p_r] = -k \frac{\partial^2 p_r}{\partial z^2},
\]

where \( a \) is the root radius, i.e. \( 2\pi a \) is the root surface area per unit length of the root. One needs to solve this equation on the domain \( z=0 \) to \( L \), where \( L \) is the length of the root, with the boundary condition \( p_r = P \) at \( z=0 \) and \( \partial p_r / \partial z = 0 \) at \( z=L \), i.e. a ‘driving’ pressure \( P \) at the base of the root \( z=0 \) and the tip of the root \( z=L \) is impermeable. It is worth noting the limiting cases for this model. If the resistance to radial flow is small compared with the resistance to axial flow, i.e. when \( (k/L^2)/2\pi a k_r \ll 1 \), then the leading-order solution is \( p_r \sim p \). In this case, the root pressure is equal to the soil pore pressure, and thus the water uptake by these types of roots is negligible. This case has been found to apply to small thin roots, such as maize side branches, which have high radial conductivity since the root cortex is thin, but low axial conductivity since the xylem vessel radii are small.\(^1\)

\(^1\)We would like to remind the reader that the axial conductivity scales as the fourth power of the root radius. Therefore, small changes in the root radius can lead to large changes in the axial conductivity.

Phil. Trans. R. Soc. A (2008)
Another limiting case is when \( (k/L^2)/2\pi ak_r \gg 1 \). In this case, we find that 
\[ \frac{\partial^2 p_r}{\partial z^2} = 0, \]
and therefore the fluid pressure inside the root is approximately uniform and equal to the driving pressure at the base, i.e. \( p_r \sim P \). This case has been found to apply to large thick roots, such as maize main roots, which have large xylem vessels in comparison with the cortex thickness. Of course, the conductivities of the root cortex and xylem are not constant in time. Instead, they depend on the levels of tissue maturation and environmental factors. However, the relationships and conclusions presented above, in principle, hold for variables that are functions of time since equation (2.6) only needs to be integrated in space and not in time. We would like to point out that, for small thin roots to become functional, one would need to increase the axial conductivity or decrease the radial conductivity or both. Thus, the early plant tissues that have not reached maturation might actually serve to make the small thin roots more functional.

The moral of these two limiting cases is that, for large-scale water uptake models, it is not entirely correct to include the volumetric sink term that is proportional to root-system length density since not all roots in the root system are actively participating in water uptake. Instead, one should only include the largest roots that have the ratio of axial to radial conductivity larger than or equal to 1, i.e. \( (k/L^2)/2\pi ak_r \geq 1 \), and the contribution of the water that comes from the sub-branches that are still influenced by the main root internal pressure (Roose & Fowler 2004b). This is in agreement with early experimental work conducted by Passioura (1972), who found that plants without side branches were able to complete their life cycle as equally well as, if not better than, plants with side branches in the situation where the water supply was limiting.

In conclusion, water uptake analysis on the single-root scale has provided us with invaluable information about the size and functionality of roots within the root system. This information will become very useful when building models for water uptake on a field scale.

\[(c)\text{ Models of root hairs} \]

In all the models for nutrient and water uptake by a single root, the root surface has been considered to be roughly flat, so that it can be approximated by a cylinder. However, most plants have root hairs near their tip. Root hairs are long and thin extensions of the root surface epidermal cells, and researchers have long pondered what they might do for a plant. One hypothesis is that root hairs increase the total surface area where nutrients may be taken up. Therefore, they might represent one of the mechanisms with which plants react to nutrient deficiency in the soil. Thus, the root hair structure and morphology can be extremely dynamic. For example, the roots can have more and longer root hairs in a loose soil than in a densely packed soil. Also, it is thought that they are dynamically renewed in response to environmental cues. All this makes the modelling of root hairs very challenging. One of the first groups to consider root hairs in their model was that led by Peter Nye (Tinker & Nye 2000). They developed a model attempting to explain experimentally obtained phosphate uptake values that were exceeding those calculated by one of the previously available models. In this case, the continuity equation for root uptake, equation (2.1), is extended with a separate sink term for nutrient influx into root hairs.
which is based on a steady-state approximation for the nutrient concentration near the root hairs. This sink term is purely phenomenological, and thus one could not use this model to confer the values of root hair uptake properties. More importantly, we would like to point out that, in most cases, the nutrient uptake properties of the root surface (as in equation (2.2)) are measured experimentally for roots with root hairs. Therefore, it is not entirely correct to say that when the model does not agree with experimental data, it is because the root hair effect has been neglected. Recently, the method of homogenization has been applied to upscale water and nutrient flow around individual root hairs to the scale of a single root in a hairy-root reactor (Ptashnyk submitted). We believe this to be a first attempt to rigorously approach this subject. While it is mathematically challenging, we believe this approach to hold great potential for future work on hairy roots in the soil. The biggest challenge here lies in translating the existing mathematical results into a language that is approachable by the experimental community.

(d) Models of soil microbiology and fungi

In addition to taking up nutrients and water from the soil, roots also exude carbon into the soil. There are thought to be several reasons for this phenomenon. First, it is thought that exudation can serve to lubricate the plant root growth through the soil. Second, exuded organic acids can interact competitively with solutes in the soil, thus leading possibly to higher levels of available nutrients to plants. Finally, the organic compounds that are exuded serve to feed the microbes, fungi, etc. that live in the soil, and this can lead to an increase in the microbial population and fungal hyphae, which can indirectly contribute to the break-up of more substantial soil organic matter and thereby increase the availability of nutrients to plants (see references in the electronic supplementary material).

Early models of the dynamics of the microbial biomass around a cylindrical root have been reviewed by Toal et al. (2000). Toal et al. (2000) pointed out that the soil microbiology models can be roughly split into two types: process-based models that consider one generic soil microbial colony that influences (bio)chemistry around a root, and organism-based models that consider the organism-oriented flow of carbon through the plant–soil continuum. As far as we can see, both of these approaches use compartmental models with differing degrees of complexity when describing the ‘flows’ between these compartments. Since the microbiology of the soil is complex, almost all of these models suffer from lack of proper input variables to be truly quantitatively predictive.

The contribution of mycorrhizae to plant nutrient uptake has been modelled by Schnepf & Roose (2006), Schnepf et al. (2008) and Landis & Fraser (2008). The most recent of these, Landis & Fraser (2008), models plant, mycorrhizal fungus and microbe interactions using in total 25 state variables in a pooled model, i.e. the model consists of 25 ordinary differential equations describing the interactions between these different pools. Thus, the model by Landis & Fraser (2008) was not spatially explicit, a fact that can have huge implications on interpreting phosphate uptake by mycorrhizae using this model. Schnepf & Roose (2006) and Schnepf et al. (2008) developed a spatially explicit model to specifically assess phosphate removal from the soil by plants with a growing mycorrhizal colony. They used a volumetric sink term that is dependent on the

Phil. Trans. R. Soc. A (2008)
surface area of the external fungal hyphae as well as the uptake capacity of the hyphae. Fungal growth in their model is described using a spatially explicit hyphal growth model that was calibrated against experimental data. However, the specifics of root–mycorrhiza infection and translocation of phosphate and carbon were not included.

Soil microbiology can undoubtedly play a major role in carbon, phosphorus and nitrogen cycling (Toal et al. 2000). However, there does not seem to be agreement on how to incorporate these effects into large-scale models. Thus, more mathematical and conceptual work in this area is needed.

(e) Root-system scale models

In the previous sections, we discussed mathematical models describing single-root scale nutrient and water uptake. Clearly, the knowledge gained should be translated from single-root scale to the plant and crop scales. In this section, we describe how the models for water and nutrient uptake on plant and crop scales are built and how the information from the single-root scale influences these models.

Models of different complexities have been used to describe the root system. The majority of root-system growth models use developmental rules that can be influenced by environmental conditions, sometimes introducing stochastic effects (see Dunbabin et al. (2002) and the chapters by Diggle and Fitter in Waisel et al. (2002)). Developmental root growth models have been strongly influenced by formulating the ‘morphogenetic programme’ of root-system development into basic growth rules (Waisel et al. 2002). Initially, the goal was to obtain a good visual/topographical agreement between observed and simulated root systems. These models have later been coupled with soil nutrient and water transport models. However, one is usually not interested in the solution of the nutrient or water uptake by a specific three-dimensional root structure. Instead, one is interested in average properties of uptake and average traits of the root system that make the most difference to the outcome. Thus, conducting three-dimensional simulations is probably not efficient in general. However, three-dimensional simulations can become valuable when answering complex scientific questions about plant root function in extreme environmental conditions and when untangling the complicated feedback loops in the root–soil continuum. In this case, the models outlined earlier are linked up to the three-dimensional structures by boundary conditions. However, we need to stress that, even with increasing computing power, the simulation tools commercially available, such as Comsol Multiphysics, are still not as well developed for three-dimensional simulations as for lower-dimensional simulations, and it is often necessary to develop bespoke computer codes for solving these problems. Thus, our view is that, before embarking on building three-dimensional computer simulation packages, the system must be analysed in full using analytical tools to justify the time and resources required for such large computational endeavours.

The best alternative to full three-dimensional simulations on a specific root structure is to use some level of averaging and homogenization to derive field-scale models. In such models, uptake of water and solutes is described by a volumetric sink term in the mass conservation equation. The art is to derive the sink term in a mathematically rigorous manner.
The equation for conservation of water in the soil is (Roose & Fowler 2004b)
\[
\frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{u} = -F_w, \tag{2.7}
\]
where \(F_w\) is the volumetric sink term for water uptake by the root system. \(F_w\) is dependent on the local root surface area per unit soil volume and the soil water saturation (Feddes et al. 2001) or water pressure inside the roots (Doussan et al. 1998), or both (Roose & Fowler 2004b; Doussan et al. 2006). Most models take \(F_w\) to be proportional to the local root length density. However, the analytical work discussed in §2b suggests that only the largest roots in the root system need to be included in this sink term.

The equation for conservation of solutes in the soil can be constructed in a similar fashion to the water uptake (Roose & Fowler 2004a), i.e.
\[
\frac{\partial}{\partial t} [(b + \theta)c] + \nabla \cdot [cu] = \nabla \cdot [D_r \nabla c] - F_s, \tag{2.8}
\]
where \(F_s\) is the volumetric sink term for solute uptake by the root system. \(F_s\) is dependent on the local root surface area per unit volume of soil and the concentration at the root surface area. Note that equation (2.8) is coupled with equation (2.7) via the volumetric water content \(\theta\). The local root surface area is sometimes computed based on a macroscopic description of the root length density or on one of the more complex root-system models described above. We would like to take this chance to point out the difference between the definition of the concentration \(c\) in the single-root scale model given by equation (2.1) and in the root-system scale model (2.8). On the single-root scale model (2.1), \(c\) is defined as an average concentration in the fluid within a representative sample of soil that does not include anything other than soil particles, fluid and air. However, the concentration \(c\) in the root-system scale model is an average concentration in the soil with roots, and thus it inherently averages out any concentration gradients around single roots. When modelling plant nutrient uptake on a root-system scale, the challenge is to further replace simplifications made by more rigorous solutions using mathematical upscaling and homogenization techniques. However, a rigorous homogenization theory for self-similar structures such as plant roots does not exist. Thus, it needs to be developed.

(f) Field-scale models within the crop growth models

Crop models are used to describe crop growth, the fate of agrochemicals in the soil–plant system, carbon and nitrogen dynamics, leaching of agrochemicals into groundwater or the effect of climate change on crop production. All these models have submodules for water and nutrient uptake. The temporal scale in these models is of the order of days or weeks and the spatial scale is on the plot, field or regional scale. Examples for crop models are ANIMO, APSIM, CENTURY, DAISY, DNDC, DSSAT, EPIC, FUSSIM2, LINTUL, MOTOR, SUNDIAL and WAVE (see references in the electronic supplementary material and also Thornley (1976) and Thornley & Johnson (1990)). Root growth and root water and solute uptake are included in these models with different degrees of complexity. At the level of the highest complexity, one-dimensional versions of equations (2.7) and (2.8) are solved. Only the root length density of a single-root system is replaced by a macroscopic root length density of the plot, which is

Phil. Trans. R. Soc. A (2008)
due to the root systems of several plants. The results are extrapolated to larger scales, sometimes by using a geographical information system or geostatistical methods. Root growth is often described by the macroscopic root length density without the details of the root branching structure, and root water and solute uptake is generally described with some kind of approximation with regard to the concentration at the root surface. Rhizodeposition is generally ignored or treated as a separate soil organic matter pool (Bruun et al. 2003). General problems inherent in these models are that the number of state variables is very high, in some cases more than 100. This makes the model analysis very cumbersome. Indeed, in scientific publications, one cannot even write down all the equations that are being solved, and thus the user is often not aware of the model assumptions and limitations. Another potential problem originates from the fact that these models need to be calibrated with numerous different parameter sets in order to be useful for applications, and thus they cannot always be relied upon to give mechanistic predictions about the behaviour of the system. To improve these models, the empirical simplifications used in them should be replaced by effective parameters based on rigorous upscaling results. This would have the benefit of opening up the use of small, laboratory, genomics and metabolomics scale experimental data to support the large-scale models.

While the theory of upscaling and homogenization of periodic structures is reasonably well established (although, as mentioned earlier, not necessarily translated by mathematicians into a language suitable for the experimental/applied community), the theory of upscaling and homogenization of nearly periodic structures that would incorporate environmental and structural stochasticity with self-similar structures is missing. However, clearly, inclusion of such variability in the models is of crucial importance if one wishes to link the models to the experimental measurements.

3. Conclusions and future avenues for research

While academic research is often portrayed as having no immediate real-world implication, a better understanding of plant–soil interactions is likely to improve the lives of a large number of people. In particular, this field has much to contribute to our understanding of climate change. The water cycle and carbon cycle obviously play important roles in climate change. Therefore, the mechanistic understanding of crop and forest growth would give invaluable insight into how they might influence the climate and how climate might influence plants. Mathematical modelling can help in developing this understanding by ensuring that the interaction between and relative importance of different mechanisms are placed on a quantitative basis.

Another obvious area in which the study of the plant–soil interaction can enhance people’s lives is agriculture. Improved mechanistic understanding of crop growth and soil management will contribute towards better management of global food supplies. Living in a developed world, it is difficult to personalize the fact that food supply is a serious, life and death, problem for many in the world. Unless steps are taken, food shortages are only going to get worse due to the increasing population and the effects of global warming on agriculture. It has recently been reported that global wheat stocks have hit an all-time low since the Second World War. These shortages and resulting price rises have in part been
attributed to droughts in Australia and China. Thus, if one is to solve the problem of food shortages in the long term, mechanistic understanding of which crop traits would do best in the future would be invaluable, and mathematical modelling can help there.

The questions that could be answered using mathematical models range from estimating the crop yields based on predicted climate data to specifying, for example, which root architecture and rhizosphere traits would perform best in different environmental conditions. However, in order to answer these questions, one needs to use mathematical models that are rigorous with truly predictive power. At present, there are two types of mathematical models that could be used to answer these questions: mechanistic mathematical models and phenomenological models.

The problems inherent in phenomenological models are that they need to be trained on large datasets and they can only make true predictions within the bounds of these datasets and their uncertainty. Another problem that one can envisage is that the phenomenological crop models tend to have a large number of state variables (perhaps over 100) and an even larger number of input parameters. If these large models are calibrated against data that have approximately the same number of data points, then one cannot really say that the model has any scientific value. In this situation, if one tweaks the parameters of these models enough, one should be able to predict every dataset. In addition, it is our experience that the fitting of the model to a ‘training dataset’ is often done by eyeballing, i.e. comparing visually the data on the computer screen against the numerical solution to the model. This is clearly not rigorous.

Mechanistic mathematical models are best for asking questions about the functioning of the systems and how the systems might respond to changes in input parameters that are derived from experiments on different spatial scales. However, the problem is that mechanistic models are much more difficult to build than phenomenological models, since they require an understanding of phenomena on different spatial scales and close collaborations between experimentalists and modellers. Clearly, it would take time to build a truly mechanistic mathematical model for the whole plant, as is currently being attempted for the human body by the Physiome Project (www.physiome.org). One might even argue that it would be almost impossible to develop such models within a single human generation. Thus, a more realistic short- and medium-term goal would be to build mechanistic models for subcomponents of the system that could be used to answer specific questions. For example, a mechanistic model for water uptake by different plants would make an invaluable contribution to the understanding of the water cycle and help to identify the root traits that would be either most robust for extreme climate events or most efficient for specific situations where water supply is scarce. While some of the mechanistic models already exist, they have unfortunately not been used to answer such mechanistic/optimization problems. This has been largely because the specialization in science in the past has led researchers to work in narrow areas of expertise. However, with the recent upsurge in collaborative science, mathematicians and experimentalists are beginning to work on an equal footing in order to answer scientific questions. However, in order to do this properly and scientifically rigorously, we need to work together in the long term and to pay careful attention to the mechanistic understanding of processes. It is always
tempting to find quick-fix solutions to big questions. However, rigorous work needs time, effort and patience, which goes beyond the standard length of the research programmes funded by most research agencies.

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References


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AUTHOR PROFILES

Tiina Roose
Tiina Roose (left) received her diploma engineering degree from the Tallinn Technical University, Estonia, in 1993 and her master’s and DPhil degrees from the University of Oxford in 1995 and 2000, respectively. In the past 10 years, she has worked in the area of mathematical biology and, in particular, on modelling plant nutrient uptake at the University of Oxford and Harvard University. She has obtained grants in the area of multiscale modelling from various funding agencies (the BBSRC, the Royal Society and the British Council). Currently, she is a Royal Society University Research Fellow at the University of Oxford.

Andrea Schnepf
Andrea Schnepf (right) received her master’s and PhD degrees in environmental engineering from BOKU–University of Natural Resources and Applied Life Sciences, Vienna, Austria, in 1999 and 2002, respectively. She received her master’s degree in applied and computational mathematics from the University of Oxford in 2005. She has obtained grants from various funding agencies (the FWF, the WWTF, the OFG and the British Council). Currently, she is a Hertha-Firnberg Fellow at the Institute of Soil Science, Department of Forest and Soil Sciences at the BOKU University. Her research interests are the mathematical modelling of plant and soil interactions and the application of these models in areas such as phytoremediation and agriculture.