NUMERICAL MODELING OF THREE-DIMENSIONAL TRANSIENT ROOT GROWTH WITH SIMULTANEOUS WATER FLOW AND NUTRIENT TRANSPORT

Plant leaves gather the sunlight and carbon dioxide from the atmosphere needed for photosynthesis. From the soil, plant roots gather the water and minerals, mostly essential but some not essential or even toxic. Feedback mechanisms in both unstressed and stressed environmental conditions control relationships between the above and below ground portion of the plant. Root growth increases the accessibility of the root system to the pool of water and nutrients, thereby enhancing plant production or plant survival in water or nutrient limiting conditions. The shape and extent of the root systems influences the rate and pattern of nutrient and water uptake from the soil. Root activities alter the pH, microbial population, chemical constituents, and structure of the soil. At the same time, root configuration is influenced by nutrient and water availability and other environmental factors such as soil temperature and soil mechanical strength. Temperature indirectly affects many root growth processes and their interactions with the surrounding rhizosphere. In turn, plants have a major modulating influence on soil temperature by altering the energy balance through shading of the soil and transpiration.

It is apparent that the shape and extent of root systems influence the rate and pattern of nutrient and water uptake from the soil. However, studies have also shown that root configuration is influenced by nutrient and water supply. For example, we know that when plants suffer from an overall deficiency of nitrogen, their roots branch more in regions where the soil is locally enriched with nitrogen fertilizer. Studies of nutrient transfer to single or widely spaced roots have shown that resistance to nutrient transfer within the soil can reduce the rate of uptake (Barley, 1970). Hence, knowledge of the configuration of the root system is important for understanding water and nutrient uptake. Other factors affecting root system morphology and distribution in a soil include (Nye & Tinker, 1977): genetic effects, time and growth stage, chemical effects (pH, salinity and toxicant concentration), soil water content, oxygen concentration, mechanical resistance, and soil temperature. However, information on the effects of many of these variables is often lacking, and the mechanisms by which they operate are largely unknown. The complex interplay among the root system, the soil, and the atmosphere can control the transfer of nutrients and natural and man-made pollutants between the soil, the plant, and ground or drainage water, and thereby affecting the exposure of humans and animals to toxicants.

Although the importance of plant root morphology seems evident for understanding root functions, there has been limited progress in quantifying and describing plant root architecture as a response of local soil environmental conditions, and how it varies between plant species, genotypes or cultivars, and within individual root systems. Moreover, classification rules describing the interactions between root growth and environmental conditions are lacking in the literature (Klepper & Rickman, 1990).

Root architecture and their dynamic responses to various soil conditions are of pivotal importance for evaluating plant growth, under both current and potential changing climatic conditions. Interactions between roots and soil in the rhizosphere can control the quantity and quality of ground water transport between the soil surface and the saturated zone, as well as exposure to human and animal life. The uptake of chemicals by vegetation leads to food chain bioaccumulation. Pesticides, PCB's, herbicides and other organic contaminants have been found to accumulate in grain crops as well as in natural vegetation. Selenium, present in soils in the western side of California's San Joaquin Valley, can accumulate to extremely high concentrations in certain plant species. Roots can intercept percolating water, thereby preventing soluble selenium from accumulating in surface and subsurface waters. Moreover, the rhizosphere might be responsible for accelerated breakdown of organic chemicals by biodegradation. These interactions have important long term consequences in the quality of our soil and water resources. Therefore, an understanding of the interactions between the roots and surrounding soil and solutes under a variety of changing environmental conditions have large implications since it can lead to a decrease in the contamination of our groundwater resource.

The mathematical modeling of root water and nutrient uptake has been simplistic to date. With the new generation of high speed computers and the availability of transient flow and transport models, we are at a cross-roads and at the verge of the capability of describing flow and transport processes at and near roots at the micro-scale in multiple dimensions. The task of describing and quantifying changes in root system architecture is not straight forward. Some researchers have focused on the form of entire root systems independent of where the roots are placed within the soil (Fitter 1985; 1986; 1987). Others have focused on the distribution of root density within soil profiles independent of the form of entire root systems (e.g. Gregory, 1988). In order to gain insight into the functional implications of an alteration in root development and root architecture it is imperative that we incorporate both methodologies. Understanding how the distribution of branching events, link elongation and branching angles within root systems change with the environment and how these changes affect the *in situ* placement of roots within the soil matrix will provide us with a more complete understanding of the responses of root systems to their environment.

Root growth models can be categorized into deterministic and stochastic models. A numerical computer model to simulate the growth of plant root systems was developed by Hackett & Rose (1972a, 1972b). Given assumptions with regard to various root growth attributes such as elongation rate and inter-branch distance, root growth was simulated, yielding total root length, root length density and age of the root system. Given certain growth responses in terms of elongation rate and branching, the effects of fertilizer treatments were studied by Lungley (1973). The impact of soil temperature on root growth for winter wheat was simulated by Porter *et al.* (1986). Subsequently, Diggle (1988) described the growth of fibrous root systems in three dimensions. This model generates a pictorial representation of the root system in which the locations of all branches and root tips are recorded in three dimensions. In a similar fashion, Pages *et al.* (1989) simulated three-dimensional root growth for a maize root system. However, as pointed out by Klepper & Rickman (1991), roots cannot be modeled without priori reference to the shoot since there are feedback

mechanisms which operate between the root and shoot. Only if the shoot is growing and functioning normally, will the roots receive the necessary growth requirements for the generation of new root length. There are feedback mechanisms for maintaining shoots and roots in relation to one another under both unstressed and stressed conditions (Brouwer, 1983).

We have made significant progress in the computer modeling of root growth. To simulate the interactive relationships between soil water/soil strength distributions and plant water uptake patterns, we have developed a three-dimensional transient root growth and water flow model, with their interface controlled by the root water uptake term (Clausnitzer & Hopmans, 1993, 1994). We considered a single plant in a covered pot to eliminate soil evaporation. The soil domain considered is discretized into a grid of finite, cuboid-shaped elements of, e.g., 1 cm side length. In addition to its spatial coordinates, each node is assigned an initial soil water potential value. Four basic, species-dependent parameters are used to describe assimilation and carbohydrate partitioning: leaf area per dry shoot mass, LA/m_s, potential transpiration per leaf area, T_{pot}/LA, water use efficiency, W, and root/shoot carbohydrate partitioning ratio, RSR. While all these four parameters may change as a function of plant age, potential transpiration per leaf area and RSR are, in addition, assumed to be directly influenced by soil environmental factors, and thus by soil strength, soil water content and temperature. This approach, implying an information pathway between root and green plant parts, is in agreement with experimental results reported by Masle & Passioura (1987), and Masle *et al.* (1990) for wheat, and Masle (1992) for barley grown under different soil strength conditions.

The mechanistic nutrient uptake models to date have serious limitations. They are basically one-dimensional and roots are considered to be smooth cylinders thus ignoring their intricate two- or three-dimensional geometry. Nutrient uptake is assumed to occur evenly along the roots, therefore the effect of root age on nutrient uptake is neglected. The roots are also assumed to be uniformly distributed in a soil medium which is homogenous and isotropic with no temporal and spatial gradients in volumetric moisture content. Hence the effect of root system

geometry on exploitation of the soil resource is neglected. The interfacing of a dynamic three-dimensional simultaneous transient nutrient and water flow with a growing root system improves existing mechanistic nutrient uptake models. Firstly, the root growth and water flow model is transient. Therefore, it will enhance the model's predictive capabilities for nutrient uptake by plants in field conditions where soil moisture content varies significantly over a period of time. Secondly, we have considered an impedance factor approach to describe the effect of local soil strength and temperature on root elongation. For each individual branch growth event, impedance factors with values between zero (inhibitive stress, no growth) and unity (no impedance) corresponding to current local conditions are multiplied with the theoretical unimpeded elongation rate that is obtained as a function of branch order and age from a genotype-specific input relationship. Thirdly, we have included in the root growth model a root branching parameter. Branching is controlled by the minimum required age for the root tissue at the branching point, the distance between subsequent branching points, and the angle of a new sub-branch with the respective base branch. An extension of the root growth model includes three-dimensional simulation of solute transport, including diffusion, dispersion and convection, and zero and first-order sink/source terms, with passive and active root solute uptake. The main reference for solute transport is Simunek *et al.* (1992).

Additional features in the present version of the model include calculation of mass balance for soil water flow and solute transport and a choice of options for calculation of the root water extraction function, with the possibility of including osmotic potential effects on water uptake rates. The root distribution function, necessary for computation of nodal water and solute sink term values, is now calculated taking into account all root segments rather than root tips only, as it was done in the earlier version. Effects of root age on water and solute extraction rates and of nutrient deficiency and toxicity on root growth have also been considered. Root solute uptake throughout the domain is lumped into nodal values of the sink term $S'(x,y,z,t)$, expressed as (Barber, 1984):

$$S' = \delta S + (1-\delta)\left(\frac{V_{max}R_d}{K_m + c}\right) \qquad (5)$$

where δ [–] is a partition coefficient, V_{max} [$ML^{-2}T^{-1}$] is the maximum uptake rate, K_m [ML^{-3}] the Michaelis-Menten constant, and R_d [L^2L^{-3}] the rooting density. The first term of the right-hand side refers to passive uptake, while the second one refers to active uptake. The rooting density function R_d is computed at each time step as:

$$R_d(x,y,z) = T_s\sigma'(x,y,z) \qquad (6)$$

where T_s, [L^2] is the total root surface at the current time and σ' [L^{-3}] is a function describing the current distribution of potential solute uptake sites within the soil domain.

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EMERGING SOIL MEASUREMENT TECHNIQUES AT THE MICROSCALE

The current understanding of water flow and contaminant transport in soils has been limited by existing measurement technologies. For example, the majority of established soil water measurement methods require an instrument to be inserted at or near the region of interest, thereby disturbing the environment being measured. Secondly, their operation allows for a limited number of 'point' measurements with each measurement representative for a soil volume which may be too small or too large, depending on the research objective. Therefore, measurements or results need to be scaled up or down so that the data can be interpreted properly for the scale of interest. In the application of the conceptual description of flow and transport we are limited to the macroscopic approach, because parameters can be measured only at the cm-scale or larger. Macropore and bypass flow are suggested as mechanisms by which accelerated breakthrough of contaminants occurs and their study requires measurements at the microscale. To better understand mechanical dispersion, diffusion, chemical and physical adsorption, degradation, and the role of immobile soil water regions, and other dynamic systems requires pore-size scale measurements.

Noninvasive, nondestructive measurement techniques are used at spatial scales of millimeters to micrometers. These methods allow observations of changing fluid phase content and solute concentration, which with increasing sophistication resolve increasingly smaller features of the pore space (Anderson & Hopmans, 1994). We present a current review of the concepts and operation of electromagnetic (EM) radiation techniques. EM methods are categorized by those employing radiography and those based on the principle of tomography. Although both methods make use of the attenuation of electromagnetic energy by the porous medium, radiography yields integrative information across the thickness of the medium (two-dimensional), whereas tomography makes use of reconstruction algorithms which resolve the internal distribution of phase content or density (three-dimensional). Both methods are used across a spectrum of frequencies (light, x- and y-rays).

In a radiographic measurement, electromagnetic radiation is passed through the investigated medium, with the transmitted portion quantified using a detection device. For a parallel, monoenergetic beam of x or γ-rays, the distribution of transmitted radiation through the medium is a function of the adsorption characteristics, and is defined by Lambert-Beer's law:

$$I_\lambda = I_{0,\lambda} \exp\left[-\int_0^x \mu_\lambda'(x)dx\right] \qquad (7)$$