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Abstract. In this paper we develop a mathematical model of a root-soil system, and also accurate and efficient finite element and finite difference algorithms for approximating this model. The goal of our work is to develop an understanding of the properties of root systems, which can be modified by using genetic engineering techniques, in order to improve the performance of plants when water availability is limited. The results of some numerical simulations are presented, which demonstrate the effectiveness of genetic and physical changes to the root-soil system.

1. Introduction.

Plants extract water from the soil through their roots and lose water to the atmosphere through their leaves in a process called transpiration. The environmental demand for water induces a reduction in the total potential of the water in the plant leaves as water evaporates from the leaves. This reduction of leaf water potential creates a potential gradient along the soil-plant-atmosphere-continuum which induces water transport from soil to roots and then through the plant to the leaves. The rate at which water moves is determined by the conductivity and potential gradient in the pathway. Very little (1 to 5%) of the water extracted by the root system is actually utilized for metabolism or growth, the vast majority (95 to 99%) simply passes through the plant and is lost to the atmosphere. Without the addition of water to the soil by irrigation or rainfall, the plant would quickly deplete its supply of water.

Within the root, water first flows through the cortex (outer layer of tissue) along the cell walls. At the endodermis, water must pass through the cell membranes because the cell wall pathway is blocked. Water again passes through the cell membrane as it leaves the endodermis and enters the stele (inner zone of the root). Within the stele water flows through xylem elements which are the water conducting vessels of the plant. The xylem is made up of dead cells in which the cell content has been removed and only the rigid cell wall remains. It is the goal of current research to identify the sites of major resistance in the root which might be modified using genetic engineering techniques, so that the overall resistance to water flow would be reduced. With an increased conductivity (reduced overall resistance), a smaller gradient in water potential will be required between the soil and plant leaves to meet the atmospheric demand for water. This will result in a more favorable leaf water status (higher water potential in the leaf) with no change in water used by

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the plant. The working hypothesis is that an improved leaf water status will result in an increased water use efficiency (amount of the plant biomass produced per unit of water used). It is apparent that all of these tissues must be explicitly considered in order that a model of water transport can assist in guiding the ongoing research.

The model we describe here is a reformulation of an earlier model defined by Anderson, Obeyesekere, and Upchurch [1], [11]. Their major assumptions, as are ours, are that the plant has a taproot, the soil is homogeneous (at least in horizontal planes), transpiration is the only driving force for water movement, and the total water potential is the sum of matric and gravitational water potentials. The major differences between the two models are that in our model the soil, very near to the root, and the cortex are assumed to be saturated, and that our model is formulated completely in terms of the water potentials.

We describe the transport of soil-water in the roots and the surrounding soil, for a given transpiration rate, by three coupled partial differential equations. The first describes water transport through the soil. In it, the roots are treated as a water sink. The second equation describes the radial flow of water into the secondary roots along the soil-cortex-endodermis-xylem path. Finally, the last equation describes the transport of water through the xylem vessels in the taproot; wherein, the secondary root system is treated as a water source. Most of the models preceding this one merely incorporated the water uptake effect through an empirically defined source function (see, e.g., [10] and [8]), although the work of [9], [7], and [11] moves in the direction of actual flow modeling. In the next section, we derive an expression for the water uptake term by considering the closed form solution of the second equation mentioned above.

In Section 3, we derive numerical procedures based on finite elements and finite differences for approximating the solution to the equations. Some convergence results are stated in the appendix, and further details of these theoretical results and theorems can be found in [3]. These results confirm that the algorithms are stable and approximate well the true solution.

Finally, in the last section, we present and discuss the results obtained from several numerical simulations. These results illustrate the influence of the various root-cell, soil, and environmental properties on the matric water potential within the taproot xylem and within the soil. Assuming that the taproot xylem potential is directly related to the leaf water potential, the results of these simulations can help genetic engineers understand the effects of these root traits in order that they can modify the roots to produce more productive plants.

2. The model.

We first consider the flow of water in the soil. It is assumed that the block of soil containing the roots (see Fig. 1) is an unsaturated homogeneous porous medium and that the macroscopic water flow is one dimensional, being in the vertical direction only. Moreover, we assume that the mass of water extracted by the subroots is macroscopically distributed throughout the medium. Suppose that the block of soil containing the root system is a cylinder of depth L and cross-sectional area A_s . Conservation of water mass combined with Darcy's law for vertical flow in soil gives Richard's equation [6] for the matric potential $\psi_s(z,t)$. If ρ is the density of water, $\theta(\psi)$ is the water content (volume of water per unit volume of soil), $K_s(\psi)$ is the conductivity of water in the soil, and g is the gravitational acceleration constant, then

(2.1)
$$\rho \frac{\partial \theta(\psi_s)}{\partial t} - \frac{\partial}{\partial z} \left(K_s(\psi_s) \left(\frac{\partial \psi_s}{\partial z} - g \right) \right) = -A_s^{-1} \mathcal{S} \quad \text{for } 0 < z < L, \ t > 0,$$

where S represents the macroscopic extraction of water by the plant's roots (defined by (2.11) or (2.14) below). To this equation we impose a flux boundary condition to model evaporation and precipitation at the surface of the ground, where z = 0, a time dependent function to model continuity of potential at the lower end, z = L, and an initial condition:

(2.2)
$$K_s\left(\frac{\partial\psi_s}{\partial z}(0,t) - g\right) = q_{\text{evap}}(t,\psi_s(0,t)) - q_{\text{prec}}(t) \quad \text{for } t > 0,$$

(2.3)
$$\psi_s(L,t) = \psi_{bot}(t) \quad \text{for } t > 0,$$

(2.4)
$$\psi_s(z,0) = \psi_s^0(z) \text{ for } 0 < z < L.$$

For consistency, $\psi_s^0(L) = \psi_{bot}(0)$. (Presumably, L is the depth of the water table and ψ_{bot} reflects saturated conditions.)



Fig. 1. A root-soil system.



Fig. 2. Cross-section of a root

For the taproot, we assume that the xylem bundles form a one dimensional saturated porous medium that contains a distributed water source term. Conservation of water implies that this source term is the same as the sink term for the flow in the soil medium. Again it is Richard's equation that governs the water potential in the taproot xylem, $\psi_x(z,t)$. If A_x is the total cross-sectional area of all the xylems in the taproot (or taproots in the soil column, if there are more than one), and \bar{K}_x is the saturated conductivity of a xylem, then we have that the axial flow through the taproot is given by

(2.5)
$$-\frac{\partial}{\partial z} \left(\bar{K}_x \left(\frac{\partial \psi_x}{\partial z} - g \right) \right) = A_x^{-1} \mathcal{S} \quad \text{for } 0 < z < L_x, \ t > 0,$$

where $L_x \leq L$ is the taproot's length. To this equation we impose a flux boundary condition representing the given transpiration rate at ground level and a no-flow condition at the lower end of the taproot:

(2.6)
$$\bar{K}_{x}\left(\frac{\partial\psi_{x}}{\partial z}(0,t)-g\right) = A_{x}^{-1}q_{\text{trans}}(t) \quad \text{for } t > 0,$$

(2.7)
$$-\bar{K}_{x}\left(\frac{\partial\psi_{x}}{\partial z}(L,t)-g\right)=0 \quad \text{for } t>0.$$

The coupling term S is calculated using the microscopic model. In the microscopic model, we consider *saturated* porous medium flow through the subroot cortex as well as through a small cylinder of soil surrounding the subroot (see Fig. 2). The conductivity of the medium changes as we go from the soil to the cortex, and a resistance to flow is encountered at the endodermis. In this model it is assumed that at a given depth, the water potential in the xylem of the taproot and the xylem of a subroot are equal (i.e., that the conductivity for axial flow in the subroot is very high). Neglecting the effects of gravity, then, the microscopic flow is restricted to the radial direction. So we consider the flow only in a cross-section of a generic subroot. Again Richard's equation governs the water potential $\psi_r(z,r,t)$ in the subroot; for each fixed z (between 0 and L_x) and t > 0, in cylindrical coordinates this is

(2.8)
$$-\frac{\partial}{\partial r} \left(r K_r(z, \psi_r) \frac{\partial \psi_r}{\partial r} \right) = 0 \quad \text{for } r_e(z) < r < r_s(z),$$

where $r_e(z)$ and $r_s(z)$ are the radii of the endodermis and of the saturated soil cylinder around the subroot, respectively, and $K_r(z, \psi_r)$ is the conductivity. This function is

$$K_r(z,\psi_r) = \begin{cases} \bar{K}_s & \text{if } r_c(z) \leq r \leq r_s(z) \\ \bar{K}_c(z) & \text{if } r_e(z) \leq r \leq r_c(z), \end{cases}$$

where \bar{K}_s and $\bar{K}_c(z)$ are the saturated conductivities of the soil and cortex, respectively, and $r_c(z)$ is the outer radius of the cortex. The boundary conditions for (2.8) are

(2.9)
$$\bar{K}_c(z)\frac{\partial\psi_r}{\partial r}(z,r_e(z),t) = \left(2\pi r_e(z)R\right)^{-1} \left(\psi_r(z,r_e(z),t) - \psi_x(z,t)\right),$$

(2.10)
$$\psi_r(z, r_s(z), t) = \psi_s(z, t),$$

representing the resistive endodermal layer and continuity of potential, respectively, where R is the resistance of the endodermis per unit length of root times the width of the endodermis. We should point out that there is a small inconsistency between the assumption of the subroot's soil cylinder being saturated and (2.10). A consistent approach would use K_s in place of \bar{K}_s in the definition of K_r ; however, the current approach seems to be adequate in practice [11].

We assume that the amount of water extracted by the subroots at a given depth is directly proportional to the total linear length of subroots contained within the block at that depth. So let $\mathcal{L}(z)$ denote the root length density function. Finally, using (2.9), the coupling term is given for t > 0 by

(2.11)
$$S(z,t) = \begin{cases} \mathcal{L}(z) A_s R^{-1} (\psi_r(z, r_e(z), t) - \psi_x(z, t)) & \text{for } 0 < z < L_x, \\ 0 & \text{for } L_x < z < L_x \end{cases}$$

Note that (2.8)-(2.10) can be solved analytically, since K_r is a piece-wise constant function (we must merely match the potential and the flux at the interface $r = r_c(z)$). The closed form of the solution at $r = r_e(z)$ is

(2.12)
$$\psi_r(z, r_e(z), t) = \frac{R}{R + c(z)} \psi_s(z, t) + \frac{c(z)}{R + c(z)} \psi_x(z, t),$$

where

(2.13)
$$c(z) = \frac{1}{2\pi} \left(\frac{1}{K_c} \ln \frac{r_c(z)}{r_e(z)} + \frac{1}{K_s} \ln \frac{r_s(z)}{r_c(z)} \right).$$

Now we can substitute this in (2.11) to obtain simply that

(2.14)
$$S(z,t) = S(z) (\psi_s(z,t) - \psi_x(z,t)) \text{ for } 0 < z < L_x, \ t > 0,$$

where

(2.15)
$$S(z) = \frac{\mathcal{L}(z)A_s}{R+c(z)}.$$

The full model is now (2.1)-(2.7) and (2.13)-(2.15).

We briefly mention two generalizations. First, instead of assuming a homogeneous soil, we can assume that the soil is homogeneous only in horizontal planes (strata). Also, the taproot can be nonhomogeneous. That is, we can allow θ , \bar{K}_x , and K_s to depend on depth z. Second, the model does not predict plant growth, but it may be imposed empirically by allowing L_x and S (i.e., \mathcal{L} , R, r_s , r_c , etc.) to depend on z.

We find it inconvenient to allow $L_x < L$, especially when L_x depends on t. As an alternative, let $L_x = L$ and set $\mathcal{L}(z) = S(z) = 0$ for $z > L_x$; the model is mathematically unchanged. In the next section, we shall assume $L_x = L$ and also that S = S(z, t).

3. Numerical Algorithms.

In this section we formulate finite element and finite difference schemes for approximating the potentials of the soil and xylem. We also present a method for improving the accuracy of the two approximate fluxes by a post-processing technique. A theoretical analysis of the approximation errors of both schemes is given in the appendix.

3.1 A finite element scheme. We begin by defining some notation and a weak form of the problem. Let $L^2(I)$, I = (0,1), denote the Hilbert space of square integrable functions,

$$L^{2}(I) = \left\{ u \mid \int_{0}^{L} u^{2} dz < \infty \right\},$$

and let (\cdot, \cdot) denote its inner product,

$$(u,v) = \int_0^L uv \, dz$$
 for any $u, v \in L^2(I)$.

Let $H^1(I) = \{ u \in L^2(I) | u' \in L^2(I) \}$ denote the standard Sobolev space of weakly differentiable functions in $L^2(I)$. Define the function spaces

$$\mathcal{V} = \left\{ v \in H^1(I) \, | \, v(L) = 0 \right\}$$
 and $\mathcal{U} = H^1(I).$

Integration by parts in z shows that if ψ_s and ψ_x constitute a solution to (2.1)–(2.7), (2.13)–(2.15), then $\psi_s(\cdot,t) \in \mathcal{V} + \psi_{bot}(t)$ and $\psi_x(\cdot,t) \in \mathcal{U}$ satisfies for any t > 0 the weak equations

$$(3.1) \qquad \left(\rho \frac{\partial \theta(\psi_s)}{\partial t}, v\right) + \left(K_s(\psi_s) \left(\frac{\partial \psi_s}{\partial z} - g\right), \frac{\partial v}{\partial z}\right) \\ = -[q_{\text{evap}}(\psi_s(0, t)) - q_{\text{prec}}]v(0) - \left(A_s^{-1}S(\psi_s - \psi_x), v\right) \quad \text{for all } v \in \mathcal{V}$$

and

(3.2)
$$\left(\bar{K}_x\left(\frac{\partial\psi_x}{\partial z}-g\right),\frac{\partial u}{\partial z}\right)$$

= $-A_x^{-1}q_{\mathrm{trans}}u(0) + \left(A_x^{-1}S(\psi_s-\psi_x),u\right)$ for all $u \in \mathcal{U}$;

the initial condition (2.4) must also be satisfied.

We discretize space and time as follows. Choose some partition $z_0 = 0 < z_1 < \cdots < z_M = L$ of I = (0, L), and let $h_i = z_i - z_{i-1}$, $h = \max_i h_i$. Choose some partition $t_0 = 0 < t_1 < \cdots < t_N = T$ of J = (0, T] for some final time of interest T, and let $\Delta t^n = t_n - t_{n-1}$. For any function u(z, t), denote $u(z, t^n)$ by $u^n(z)$ and let the backward time difference operator be given by

$$\partial_t u^n = \frac{u^n - u^{n-1}}{\Delta t^n}$$

Finally, let \mathcal{V}_h and \mathcal{U}_h be standard finite element subspaces of \mathcal{V} and \mathcal{U} defined over the given partition of I (see, e.g., [4]).

Our finite element procedure is the following: For n = 1, ..., N, let $\Psi_s^n \in \mathcal{V}_h + \psi_{bot}^n$ and $\Psi_x^n \in \mathcal{U}_h$ satisfy

(3.3)
$$\left(\rho\partial_t\theta(\Psi_s)^n, v\right) + \left(K_s(\Psi_s^n)\left(\frac{\partial\Psi_s^n}{\partial z} - g\right), \frac{\partial v}{\partial z}\right)$$

= $-[q_{\text{evap}}^n(\Psi_s^n(0)) - q_{\text{prec}}^n]v(0) - \left(A_s^{-1}S^n(\Psi_s^n - \Psi_x^n), v\right)$ for all $v \in \mathcal{V}_h$

and

(3.4)
$$\left(\bar{K}_x \left(\frac{\partial \Psi_x^n}{\partial z} - g \right), \frac{\partial u}{\partial z} \right)$$

= $-A_x^{-1} q_{\text{trans}}^n u(0) + \left(A_x^{-1} S^n (\Psi_s^n - \Psi_x^n), u \right) \text{ for all } u \in \mathcal{U}_h,$

where we initialize the scheme by choosing some reasonable approximation $\Psi_s^0 \in \mathcal{V}_h + \psi_{bot}^0$ to ψ_s^0 . For example, one can take the interpolant of ψ_s^0 in $\mathcal{V}_h + \psi_{bot}^0$.

One of the important quantities of interest to the agricultural scientist is the water flow rate up the taproot, which we denote by γ_x :

(3.5)
$$\gamma_x = \bar{K}_x \left(\frac{\partial \psi_x}{\partial z} - g \right).$$

For $i \ge 1$, we multiply (2.5) by $z - z_{i-1}$ and integrate in space over (z_{i-1}, z_i) to obtain with (2.14) that

(3.6)
$$\gamma_{\boldsymbol{x}}(z_{\boldsymbol{i}},t)\,h_{\boldsymbol{i}} = \int_{z_{\boldsymbol{i}-1}}^{z_{\boldsymbol{i}}} \bar{K}_{\boldsymbol{x}}\left(\frac{\partial\psi_{\boldsymbol{x}}}{\partial z} - g\right)\,dz - \int_{z_{\boldsymbol{i}-1}}^{z_{\boldsymbol{i}}} A_{\boldsymbol{x}}^{-1}S\big(\psi_{\boldsymbol{s}} - \psi_{\boldsymbol{x}}\big)(z - z_{\boldsymbol{i}-1})\,dz.$$

This motivates the definition [5], [12], [13] of our improved approximate flux $\Gamma_{x,i}^n$:

(3.7)
$$\Gamma_{x,i}^{n} h_{i} = \int_{z_{i-1}}^{z_{i}} \bar{K}_{x} \left(\frac{\partial \Psi_{x}^{n}}{\partial z} - g \right) dz - \int_{z_{i-1}}^{z_{i}} A_{x}^{-1} S^{n} \left(\Psi_{s}^{n} - \Psi_{x}^{n} \right) (z - z_{i-1}) dz.$$

In an entirely similar way, we can also approximate the water flow rate in the soil column. We define

(3.8)
$$\gamma_s = K_s(\psi_s) \left(\frac{\partial \psi_s}{\partial z} - g \right),$$

and we note that for $i \ge 1$, if we multiply (2.1) by $z - z_{i-1}$ and integrate in space over (z_{i-1}, z_i) , we obtain with (2.14) that

(3.9)
$$\gamma_{s}(z_{i},t)h_{i} = \int_{z_{i-1}}^{z_{i}} \rho \frac{\partial \theta(\psi_{s})}{\partial t} (z-z_{i-1}) dz + \int_{z_{i-1}}^{z_{i}} K_{s}(\psi_{s}) \left(\frac{\partial \psi_{s}}{\partial z} - g\right) dz + \int_{z_{i-1}}^{z_{i}} A_{s}^{-1} S(\psi_{s} - \psi_{x}) (z-z_{i-1}) dz.$$

Therefore we define our improved approximate flux $\Gamma_{s,i}^n$ by

(3.10)
$$\Gamma_{s,i}^{n} h_{i} = \int_{z_{i-1}}^{z_{i}} \rho \partial_{t} \theta(\Psi_{s})^{n} (z - z_{i-1}) dz + \int_{z_{i-1}}^{z_{i}} K_{s}(\Psi_{s}^{n}) \left(\frac{\partial \Psi_{s}^{n}}{\partial z} - g\right) dz + \int_{z_{i-1}}^{z_{i}} A_{s}^{-1} S^{n} (\Psi_{s}^{n} - \Psi_{x}^{n}) (z - z_{i-1}) dz.$$

These quantities can be computed easily from the approximate solutions of the xylem and soil potentials. They are more accurate than simply taking the fluxes directly from the approximate potentials (see the theoretical results in the appendix for a justification of this statement).

3.2 A finite difference scheme. We define a finite difference scheme (see (3.14)–(3.17) below) as a special case of our finite element scheme by specifying a certain choice for the \mathcal{V}_h and \mathcal{U}_h , and by requiring certain quadrature rules in the evaluation of the integrals. We take as finite dimensional subspaces the continuous, piecewise linear functions defined on the given mesh; that is, $\mathcal{V}_h = \operatorname{span}\{w_i\}_{i=0}^{M-1}$ and $\mathcal{U}_h = \operatorname{span}\{w_i\}_{i=0}^M$, where

$$w_i(z) = \begin{cases} (z - z_{i-1})/h_i & \text{if } i > 0 \text{ and } z_{i-1} \le z \le z_i, \\ (z_{i+1} - z)/h_{i+1} & \text{if } i < M \text{ and } z_i \le z \le z_{i+1}, \\ 0 & \text{otherwise.} \end{cases}$$

We use the midpoint rule to evaluate any integral involving a spatial derivative, and otherwise we use the trapezoidal rule. We denote these rules, respectively, as discrete inner products for any u and v as

$$\langle u, v \rangle_{\mathcal{M}} = \sum_{i=1}^{M} u_{i-1/2} v_{i-1/2} h_i$$
 and $\langle u, v \rangle_{\mathcal{T}} = \frac{1}{2} \sum_{i=1}^{M} (u_i v_i + u_{i-1} v_{i-1}) h_i$

where we use the notation $u_i = u(z_i)$, $z_{i-1/2} = (z_i + z_{i-1})/2$, and $u_{i-1/2} = u(z_{i-1/2})$. Note that for $u \in U_h$ or \mathcal{V}_h , $u_{i-1/2} = (u_i + u_{i-1})/2$.

Our finite difference procedure is then the following: For n = 1, ..., N, let $\Psi_s^n \in \mathcal{V}_h + \psi_{bot}^n$ and $\Psi_x^n \in \mathcal{U}_h$ satisfy

$$(3.11) \quad \langle \rho \partial_t \theta(\Psi_s)^n, w_i \rangle_{\mathrm{T}} + \left\langle K_s(\Psi_s^n) \left(\frac{\partial \Psi_s^n}{\partial z} - g \right), \frac{\partial w_i}{\partial z} \right\rangle_{\mathrm{M}} \\ = -[q_{\mathrm{evap}}^n(\Psi_s^n(0)) - q_{\mathrm{prec}}^n] \delta_{i,0} - \langle A_s^{-1} S^n(\Psi_s^n - \Psi_x^n), w_i \rangle_{\mathrm{T}} \\ \text{for } i = 0, 1, ..., M - 1,$$

and

(3.12)
$$\left\langle \bar{K}_{x}\left(\frac{\partial\Psi_{x}^{n}}{\partial z}-g\right),\frac{\partial w_{i}}{\partial z}\right\rangle_{\mathrm{M}} = -A_{x}^{-1}q_{\mathrm{trans}}^{n}\delta_{i,0} + \langle A_{x}^{-1}S^{n}(\Psi_{s}^{n}-\Psi_{x}^{n}),w_{i}\rangle_{\mathrm{T}}$$

for $i = 0, 1, ..., M$,

where $\delta_{i,j}$ is the Kronecker delta. We initialize the scheme by choosing the interpolant of ψ_s^0 :

(3.13)
$$\Psi^{0}_{s,i} = \psi^{0}_{s,i} \quad \text{for } i = 0, 1, ..., M.$$

Our scheme can be expressed equivalently in more traditional finite difference notation as follows. We first define by reflection $h_0 = h_1$, $h_{M+1} = h_M$,

$$\psi_{s,-1} = \psi_{s,1} - 2gh_1, \quad \psi_{x,-1} = \psi_{x,1} - 2gh_1, \quad \psi_{x,M+1} = \psi_{x,M-1} + 2gh_M,$$

and $K_s(\Psi_{s,-1/2}^n) = K_s(\Psi_{s,1/2}^n).$

Then, for n = 1, ..., N and i = 0, ..., M, let $\Psi_{s,i}^n$ and $\Psi_{x,i}^n$ satisfy

(3.14)
$$\Psi^{0}_{s,i} = \psi^{0}_{s,i}$$

$$(3.15) \qquad \Psi_{s,M}^n = \psi_{\rm bot}^n$$

(3.16)
$$\rho \partial_t \theta(\Psi_{s,i})^n - \frac{2}{h_{i+1} + h_i} \bigg[K_s(\Psi_{s,i+1/2}^n) \bigg(\frac{\Psi_{s,i+1}^n - \Psi_{s,i}^n}{h_{i+1}} - g \bigg) \\ - K_s(\Psi_{s,i-1/2}^n) \bigg(\frac{\Psi_{s,i}^n - \Psi_{s,i-1}^n}{h_i} - g \bigg) \bigg] \\ = -\frac{2}{h_1} [q_{\text{evap}}^n(\Psi_{s,0}^n) - q_{\text{prec}}^n] \delta_{i,0} - A_s^{-1} S_i^n(\Psi_{s,i}^n - \Psi_{x,i}^n) \quad \text{if } i \neq M,$$

(3.17)
$$-\frac{2\bar{K}_{x}}{h_{i+1}+h_{i}}\left(\frac{\Psi_{x,i+1}^{n}-\Psi_{x,i}^{n}}{h_{i+1}}-\frac{\Psi_{x,i}^{n}-\Psi_{x,i-1}^{n}}{h_{i}}\right)$$
$$=-\frac{2}{h_{1}}A_{x}^{-1}q_{\text{trans}}^{n}\delta_{i,0}+A_{x}^{-1}S_{i}^{n}(\Psi_{s,i}^{n}-\Psi_{x,i}^{n}).$$

We can also define the improved fluxes by the same choice of quadrature rules: the midpoint rule on integrals involving spatial derivatives and the trapezoidal rule otherwise. From (3.7) and (3.10), we therefore define for i = 1, ..., M,

(3.18)
$$\Gamma_{x,i}^{n} = \bar{K}_{x} \left(\frac{\Psi_{x,i} - \Psi_{x,i-1}}{h_{i}} - g \right) - \frac{1}{2} A_{x}^{-1} S_{i}^{n} \left(\Psi_{s,i} - \Psi_{x,i} \right) h_{i}$$

(3.19)
$$\Gamma_{s,i}^{n} = \frac{1}{2} \rho \partial_{t} \theta(\Psi_{s,i})^{n} h_{i} + K_{s}(\Psi_{s,i-1/2}^{n}) \left(\frac{\Psi_{s,i} - \Psi_{s,i-1}}{h_{i}} - g\right) \\ + \frac{1}{2} A_{s}^{-1} S_{i}^{n} (\Psi_{s,i} - \Psi_{x,i}) h_{i}.$$

3.3 Remarks on implementing the schemes. Our two schemes are nonlinear, so some iterative procedure such as Newton's method or a Picard successive substitution must be used to solve the equations. (The results of the next section were obtained from a finite difference code utilizing a Newton iteration procedure.) If we order the unknowns spatially, alternating the two potentials, we obtain a block tridiagonal system; the blocks are 2×2 . As a consequence, direct Gaussian elimination can be used effectively to solve the matrix problems that arise.

4. Simulation Results.

The data used for the standard, base case in the simulations is given in Table 1, wherein r_t is the radius of a single taproot xylem and N_t is the total number of taproot xylems in the soil block (thus $A_x = N_t \pi r_t^2$), and also μ is the water viscosity and \bar{K}_x is defined from the Hagen-Poiseuille law for fluid flow through pipes (i.e., $\bar{K}_x = \rho r_t^2/8\mu$). We used the finite difference scheme to obtain the results discussed

Quantity	Value (in S.I. units)
L	1
A_s	4
r_t	.0005
N_t	150
$\mathcal{L}(z)$	10(1-z) + .0005
R	$2 imes 10^8$
r_e	.00022
r_c	.005
r_s	.02
\bar{K}_s	0.58
\bar{K}_c	15
$q_{\mathtt{trans}}(t)$	$\max(.0013\sin(\pi t/43200), 0)$
$q_{\tt evap}$	0
$q_{\sf prec}$	0
$K_s(\psi)$	$[3.56(-\psi/2350)^{(-12.2/10.9)} - 1.09] \times 10^{-7}$
$ heta(\psi)$	$-\ln(-\psi/2350)/10.9$
$\psi^0_s(z)$	-709.8 + 9.8z
$\psi_{ extsf{bot}}$	-700
ρ	1000
μ	10 ⁻⁶
g	9.8
h	2 ⁻⁹
Δt	42.1875

TABLE 1.Simulation parameters.

in this section. Note that since the initial soil potential is linear, the initialization of our finite difference scheme is exact.

Our initial condition assumes that the root-soil system is at equilibrium at 6:00 a.m., just before transpiration begins. We let the transpiration rate follow the positive portion of a sine curve from 6:00 a.m. to 6:00 p.m.; thereafter, transpiration is set to zero.

The first three figures, Fig. 1(a), 1(b), and 1(c), show hourly potential profiles of the soil. Back flow occurs during the latter part of the day, recharging the soil matrix near the surface. Compared to the soil profiles, Fig. 2(a), 2(b), and 2(c) illustrate that the xylem potential is very low, and that it varies dramatically in time, but very little in space (see Fig. 3(a) for a comparison to the first three figures on the same scale).

In the following discussion, the potentials are given at noon, and data varying from that given in Table 1 is noted in the figures. During transpiration, production is hampered by the low xylem potential at z = 0, since it is related directly to the leaf potential. In order to obtain a more favorable xylem potential, we first discuss some non-genetic changes, shading and tilling. We simulate these two processes by changing the transpiration rate and the conductivity of the soil, respectively. As seen by Fig. 3(a), 3(b), 4(a), and 4(b), shading (decreased amplitude) shows a better ratio of decreasing the xylem potential than tilling (increased soil conductivity). However, a reduced transpiration lowers the amount of water available to the plant.

With respect to genetic changes, we consider changing the resistance and/or the thickness of the endodermis and the saturated conductivity of the cortex. Though cortex effects are negligible (Fig. 5(a) and 5(b)), the endodermis changes show profound effects on the xylem (Fig. 6–7). Recall that R is the product of endodermal resistance and thickness, so changing either one simply has the effect of changing R. It is important to realize that the transpiration rate is left unchanged when these genetic changes are made.

In conclusion, based on the simulation results of this model, genetic changes can produce dramatic reduction in xylem potential. This in turn should result in improved plant growth.



Fig. 1(a). Soil potential profiles from 6:00 a.m. to noon, base case.



Fig. 1(b). Soil Potential profiles from 1:00 p.m. to 6:00 p.m., base case.



Fig. 1(c). Soil potential profiles from 7:00 p.m. to midnight, base case.



Fig. 2(a). Xylem potential profiles from 6:00 a.m. to noon, base case.



Fig. 2(b). Xylem potential profiles from 1:00 p.m. to 6:00 p.m., base case.



Fig. 2(c). Xylem potential profiles from 7:00 p.m. to midnight, base case.



Fig. 3(a). Effects of soil conductivity on xylem potential, at noon.



Fig. 3(b). Effects of soil conductivity on soil potential, at noon.



Fig. 4(a). Effects of transpiration on xylem potential, at noon.



Fig. 4(b). Effects of transpiration on soil potential, at noon.



Fig. 5(a). Effects of cortex conductivity on xylem potential, at noon.



Fig. 5(b). Effects of cortex conductivity on soil potential, at noon.



Fig. 6(a). Effects of endodermis thickness on xylem potential, at noon.



Fig. 6(b). Effects of endodermis thickness on soil potential, at noon.



Fig. 7(a). Effects of endodermis resistance on xylem potential, at noon.



Fig. 7(b). Effects of endodermis resistance on soil potential, at noon.

Appendix.

In this appendix, we summarize the authors' main theoretical results concerning the convergence of the solutions of the approximation schemes to the true solution. Full proofs of the theorems below are given in [3]. See also the analysis of approximation errors as given by the authors in [2] for a model similar to the one in this paper (essentially the unreformulated model [11] was treated).

We use the definitions and notation given in previous sections. Also let $\Delta t = \max_{n} \Delta t^{n}$. Denote the $H^{k}(I)$ -norm by $\|\cdot\|_{k}$; that is, $\|u\|_{0} = (u, u)^{1/2}$ and, for integer $k \geq 1$,

$$||u||_{k}^{2} = \sum_{j=0}^{k} \left\| \frac{d^{j}u}{dz^{j}} \right\|_{0}^{2}.$$

Then the Sobolev space $H^{k}(I) = \{u \mid ||u||_{k} < \infty\}$ (and $L^{2}(I) = H^{0}(I)$). Finally,

$$L^{2}(J; H^{k}(I)) = \left\{ u \, \big| \, \int_{0}^{T} \|u\|_{k}^{2} \, dt < \infty \right\}$$

and

$$L^{\infty}(J; H^{k}(I)) = \left\{ u \, \big| \, \underset{t \in J}{\operatorname{ess sup}} \| u \|_{k} < \infty \right\}.$$

We make the following assumptions, wherein c and C are some fixed positive constants.

- (A1) $c \leq K_s \leq C$, $|K'_s| \leq C$, $|K''_s| \leq C$, and $c \leq K_x \leq C$.
- (A2) $0 \le S \le C, c \le S$ for z in some fixed nonempty interval for each $t \in J$, and $|\partial S/\partial t| \le C$.
- (A3) There exists some fixed integer $p \ge 2$, such that

$$\inf_{v \in \mathcal{V}_h} \|\psi - v\|_1 \le C \|\psi\|_p h^{p-1} \quad \text{for any } \psi \in \mathcal{V} \cap H^p(I),$$
$$\inf_{u \in \mathcal{U}_h} \|\psi - u\|_1 \le C \|\psi\|_p h^{p-1} \quad \text{for any } \psi \in \mathcal{U} \cap H^p(I).$$

- (A4) ψ_s , $\partial \psi_s / \partial t$, and $\psi_x \in L^2(J; H^p(I))$.
- (A5) $\partial \psi_s / \partial t \in L^{\infty}(J; H^2(I))$ and $\partial^2 \psi_s / \partial t^2 \in L^2(J; L^2(I))$.
- (A6) $|q_{\text{evap}}| \leq C, |q_{\text{prec}}| \leq C, |q_{\text{trans}}| \leq C, 0 \leq \partial q_{\text{evap}}/\partial \psi \leq C, |\partial^2 q_{\text{evap}}/\partial \psi^2| \leq C, |\partial q_{\text{evap}}/\partial \psi^2| \leq C, |\partial q_{\text{evap}}/\partial \psi^2| \leq C, |\partial^2 q_{\text{evap}$
- (A7) $c \leq h_{i+1}/h_i \leq C$ and $\Delta t^{n+1}/\Delta t^n \leq \overline{C}$.
- (A8) $\dot{\psi}_{bot} \leq 0$ and $\psi_s^0 \in H^p(I)$. Moreover, Ψ_s^0 is defined so that $\|\Psi_s^0 \psi_s^0\|_j \leq C \|\psi_s^0\|_p h^{p-j}, j = 0, 1.$
- (A9) $c \leq \theta' \leq C$ and $|\theta''| \leq C$ (physically, this means that $-C \leq \psi_s \leq -c$).

Note that (A8) is easily satisfied by reasonable initialization procedures.

We remark that θ' is in general a degenerate function: $\theta'(\psi_s) = 0$ precisely when $\psi_s \geq 0$ (the saturated region) and $\theta'(\psi_s) \to 0$ as $\psi_s \to -\infty$ (the dry region) [6]. Since most plants die in cases of either extreme, we have restricted ourselves to the case defined by (A9) above.

First, we consider errors in the finite element approximations.

THEOREM 1. Assume (A1)-(A9). Then for the solution to the finite element scheme, for h and Δt sufficiently small,

$$\begin{array}{l} \text{(i)} & \max_{n} \|\Psi_{s}^{n} - \psi_{s}^{n}\|_{0} + \max_{n} \|\Psi_{x}^{n} - \psi_{x}^{n}\|_{0} \leq C\left\{h^{p} + \Delta t\right\}, \\ \text{(ii)} & \max_{n} \left\|\frac{\partial}{\partial z}(\Psi_{s}^{n} - \psi_{s}^{n})\right\|_{0}^{1} + \max_{n} \left\|\frac{\partial}{\partial z}(\Psi_{x}^{n} - \psi_{x}^{n})\right\|_{0} \leq C\left\{h^{p-1} + \Delta t\right\}, \\ \text{(iii)} & \left(\sum_{n=1}^{N} \|\partial_{t}(\Psi_{s} - \psi_{s})^{n}\|_{0}^{2}\Delta t^{n}\right)^{1/2} \leq C\left\{h^{p-1} + \Delta t\right\}, \\ \text{(iv)} & \max_{n} \left|\Gamma_{x,i}^{n} - \gamma_{x,i}^{n}\right| \leq C\left\{h^{p} + \Delta t\right\}, \\ \text{(v)} & \left(\sum_{n=1}^{N} \left|\Gamma_{s,i}^{n} - \gamma_{s,i}^{n}\right|^{2}\Delta t^{n}\right)^{1/2} \leq C\left\{h^{p-1} + \Delta t\right\}, \end{array}$$

where C depends on the bounds in the assumptions but is independent of h and Δt , and where i = 1, ..., M. Moreover, if the scheme is initialized by setting $\Psi_s^0 \in \mathcal{V}_h + \psi_{bot}^0$ such that

$$\left(K_{s}(\psi_{s}^{0})\left(\frac{\partial\Psi_{s}^{0}}{\partial z}-\frac{\partial\psi_{s}^{0}}{\partial z}\right),\frac{\partial v}{\partial z}\right)=0 \quad \text{for } v \in \mathcal{V}_{h},$$

then h^p replaces h^{p-1} in (iii) and (v).

Note that the error in the improved xylem flux (iv) is less than that in the derivative of the xylem potential itself (ii). The same is true for the improved soil flux, since the norm in (v) is stronger than that in (ii); a careful initialization makes the improvement even better.

For the approximation error in the finite difference scheme, we obtain the following theorem, in which some of the errors are expressed in terms of the piecewise linear interpolants of the approximation's nodal values.

THEOREM 2. Assume (A1)-(A9) with p = 2. Assume also that ψ_s and ψ_x are continuous. Then for h and Δt sufficiently small, (i)-(v) of Theorem 1 hold (with p = 2) for the solution to the finite difference scheme, where again C depends on the bounds in the assumptions but is independent of h and Δt , and i = 1, ..., M. Moreover, if the finite difference scheme is initialized by setting $\Psi_s^0 \in \mathcal{V}_h + \psi_{bot}^0$ such that

$$\left\langle K_s(\psi_s^0) \left(\frac{\partial \Psi_s^0}{\partial z} - \frac{\partial \psi_s^0}{\partial z} \right), \frac{\partial w_i}{\partial z} \right\rangle_{\mathbf{M}} = 0 \quad \text{for } i = 0, 1, ..., M - 1.$$

then h^2 replaces h in (iii) and (v).

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