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Design of Porous Media for Optimal Gas and Liquid Fluxes to Plant Roots

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ABSTRACT

The selection of plant growth media remains an empirical endeavor often focusing on available materials rather than on the physical principles that govern water retention and flow. Apparent water- and O_2 -induced stresses affecting plant growth experiments in microgravity (10^{-3} – $10^{-6} g_0$) have prompted the need for refinement of selection criteria for optimal growth media. The objective of this work was to develop a comprehensive approach for selecting the physical characteristics of plant growth media that optimize the dynamic availability of liquids and gases to plant roots. Physically based models describing the relationship between content and fluxes of liquids and gases were written in terms of media parameters and were used to cast a multi-objective optimization problem. Plant physiological target values, growth container design, and other system considerations provided constraints for the optimization problem. The optimized media parameters designated a pore-size distribution (psd) that is scaled to a corresponding particle-size distribution (PSD) by inversion of the Arya and Paris model. The iterative process resulted in an average scaling of psd to PSD and led to the synthesis of an optimal medium. Sand and glass bead mixtures were well matched to the optimized media characteristics resulting from the optimization procedure. This methodology is amenable to horticultural, greenhouse, and research applications where optimal porous media design is of value.

THE DISTRIBUTION AND MOVEMENT of liquids and gases in porous media are controlled primarily by the

media pore sizes (which are functions of particle sizes and their arrangement) and driving forces or gradients. Researchers have attempted to provide optimum plant growth media for container-grown plants by characterizing the physical properties of different media (Spomer, 1974; Beardsell et al., 1979; Milks et al., 1989a,b). The limited volume and surface area of containerized growth media create intensive growth conditions for plants, increasing the need for better environmental controls (i.e., liquids and gases). The relatively narrow range of potting media particle sizes in horticultural practice arises from the need for adequate aeration provided by gravitational water being readily removed from large pores (Bunt, 1961, 1988; Handreck, 1983). In the presence of microscale accelerational forces (microgravity) aboard an earth-orbiting spacecraft, however, the maintenance of an optimal plant growth environment in porous media has sparked a set of new research questions.

Plants are proposed as part of a bioregenerative life support system for long-duration space missions, removing CO_2 and providing O_2 and potable water from transpiration and ultimately becoming a source of food (Bugbee and Salisbury, 1989; Olson et al., 1988). This research was initiated to address the question of how to optimally supply water, nutrients, and gases through porous media in microgravity, where capillary forces dominate and body forces are generally negligible (Wachinski and Preston, 1990; Antar and Nuotio-Antar, 1993). Researchers have proposed and tested systems for supplying water and nutrients to plants in reduced-gravity fields (Wright et al., 1988; Dreschel and Sager, 1989; Ivanova and Dandolov, 1992; Morrow et al., 1992,

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1993, 1994; Podolsky and Mashinsky, 1994). Despite a number of plant growth experiments in microgravity, providing an ideal stress-free growing environment for plants in space remains a challenge (Bingham et al., 1996a). Past microgravity experimental results combined with existing fundamental terrestrial research relating fluid behavior in porous media were foundational in establishing a preliminary basis for this work. A similar methodology also has application to containerized growth media for terrestrial greenhouse (Heinen, 1997) and research purposes, as well as other specialized porous media applications.

The objectives of this study were to: (i) present a methodology for selecting a plant growth medium that optimizes the fluxes of liquids and gases to plant roots using physically based parametric models that describe media properties, and (ii) use the results of the optimization to physically construct or synthesize the media and verify the optimality of the media properties.

Because of the uncertainty of fluid gradients within the porous media, we selected hydraulic conductivity and gas diffusion as surrogate flux terms. Matric head or energy considerations with regard to the control of media-water status must be considered when optimizing media properties. The properties that describe the psd of the optimal media are used to determine PSD by inversion of a particle-to-pore scaling technique, a key to the success of the proposed methodology. Optimized media parameters contribute significantly to the maximization of gas and liquid fluxes. Optimization results will be largely bound by specification of matric head constraints and by rapidly reduced gas concentrations at high water contents.

THEORETICAL CONSIDERATIONS

In this study we considered the problem of specifying optimal media properties for plant growth in a root module or

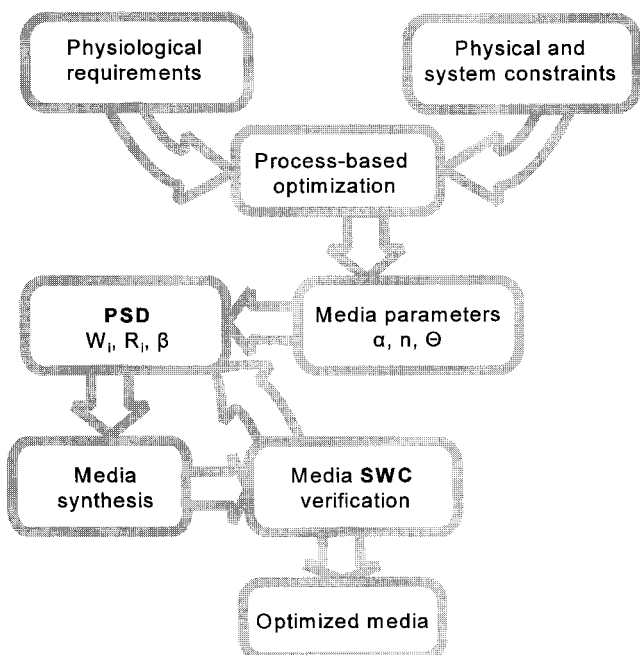


Fig. 1. Framework of the optimization and media synthesis procedure; PSD is particle-size distribution and SWC is the substrate-water characteristic.

container where water is supplied or maintained by suction-controlled porous membranes in contact with the growth medium. Such a system was found by Jones and Or (1997) to be capable of maintaining quasi-steady-state conditions when porous membrane and media properties were properly matched. In their study, unit hydraulic gradients and near-atmospheric levels of O₂ were maintained in root modules for more than 80 d of plant growth. Our analysis was therefore based on the assumption of one-dimensional steady-state conditions to simplify and facilitate analytical solutions to the problem. Due to complications in resolving the full picture of liquid and gas gradients within porous media and to simplify the optimization problem, the unsaturated hydraulic conductivity and soil gas diffusion terms serve as “surrogate” fluxes in the optimization. Hysteresis effects are not addressed in this work and therefore only the drying substrate-water characteristic (SWC) is used.

An outline of the methodology is shown in Fig. 1 where plant physiological requirements, container geometry, and water control system design form optimization constraints. Physically based and parametric models written in terms of media properties describe relationships between content and fluxes of liquids and gases and were used to cast a multiobjective optimization problem. Optimized media parameters were used to determine PSD from the relationship between pore size and particle size. Finally, the medium was synthesized and its SWC was measured to determine optimality of the porous medium based on the optimized media parameters. The usefulness of this methodology lies in the ability to express contents and fluxes of liquids and gases in terms of a few media parameters and subsequently to correctly scale psd to PSD, leading to media synthesis. We discuss the elements and relationships illustrated in Fig. 1 below.

Liquid-Phase Relationships

The foundation of liquid behavior within porous media lies in the media’s pore structure, which provides a basis for modeling liquid behavior. The SWC, which contains information on the psd, and the unsaturated hydraulic conductivity functions are necessary to express the steady-state liquid content and fluxes. Any of the two- and three-parameter models describing the SWC could be incorporated in this methodology (Brooks and Corey, 1964; van Genuchten, 1980; Kosugi, 1994; Perfect et al., 1996; Perrier et al., 1996). The SWC and hydraulic conductivity models of van Genuchten (1980) were selected due to their wide acceptance and common parameters. The van Genuchten (1980) SWC model can be expressed in terms of dimensionless water content, Θ , as a function of matric head, h (m):

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + (\alpha h)^n} \right]^{(n-1)/n} \quad [1]$$

where α (m⁻¹) and n are empirical parameters. Saturated water content is θ_s (m³ m⁻³) and θ_r (m³ m⁻³) is the residual water content. Hereinafter we refer to h as a positive value (i.e., larger h indicates a more negative matric potential).

The relative hydraulic conductivity, K_r , is defined as the ratio of unsaturated hydraulic conductivity, K (m s⁻¹), to the saturated hydraulic conductivity, K_s (m s⁻¹). The initial estimate of K_r appears to have little impact in this work where relative terms are used; however, there may be applications where estimation of K_s , a priori, is necessary. In this case, expressions relating porosity and particle diameter may be used to provide estimates of K_s (see Appendix B for discussion). The value of K_r may be expressed in terms of Θ and n using van Genuchten’s (1980) equation and Mualem’s (1976) theory as

$$K_r = \Theta^{0.5} \left[1 - \left(1 - \Theta^{n/(n-1)} \right)^{(n-1)/n} \right]^2 \quad [2]$$

Equation [1] is foundational in that it contains both the media parameters that will be optimized and water content, which governs both gaseous and liquid fluxes. Equation [2], the relative hydraulic conductivity, is used as a surrogate for the liquid flux due to the uncertainty of the hydraulic gradient, and to simplify the optimization problem.

Gaseous-Phase Relationships

Composition of different gases, i.e., O₂ and CO₂, are influenced by biological activity and the rate of gaseous exchange with the atmosphere. The general equation for gas diffusion in porous media in the presence of sinks (e.g., O₂ consumption from microorganism or plant root respiration) or sources (e.g., CO₂ production) is a combination of Fick's law with conservation of mass:

$$\phi \frac{\partial C_G}{\partial t} = D_G^s \frac{\partial^2 C_G}{\partial x^2} + R \quad [3]$$

where ϕ is air-filled porosity (m³ m⁻³), C_G (g m⁻³) is the gas concentration, t (s) is time, D_G^s (m² s⁻¹) is the gas diffusion coefficient in the substrate, x (m) is a flow path vector, and R (g m⁻³ s⁻¹) is the gas source or sink rate per unit volume (positive sign for CO₂ and negative for O₂). This equation describes the changes in gas concentration (or partial pressure) in time and space.

For steady-state gas diffusion in which $\partial C_G / \partial t = 0$, Eq. [3] reduces to

$$\frac{d^2 C_G}{dx^2} + \frac{R}{D_G^s} = 0 \quad [4]$$

Van Bavel (1951) presented solutions for Eq. [4] for a constant and uniform production-consumption rate of gas in a soil underlain by a water table at $x = L$ (an impervious boundary for gas diffusion) and an atmospheric concentration, C_o (g m⁻³), at the soil surface. Assuming D_G^s is constant with depth, we integrated Eq. [4] twice and applied the boundary conditions of Van Bavel (1951), giving the steady-state solution for the gas concentration distribution in the media profile:

$$C_G(x) = C_o + \frac{R}{D_G^s} \left(Lx - \frac{x^2}{2} \right) \quad [5]$$

The substrate gas diffusion coefficient, D_G^s , can be represented using the Millington and Quirk (1959, 1960) equation, given by

$$D_G^s = D_G^A \frac{\phi^{10/3}}{\eta^2} \quad [6]$$

in which D_G^A (m² s⁻¹) is the gas diffusion coefficient in free air and η (m³ m⁻³) is the absolute porosity of the medium. A discussion of estimating porosity based on binary mixtures is presented in Appendix B. For simplicity, we made a substitution for ϕ using $\eta(1 - \Theta)$. While this substitution may produce an overestimation of gas diffusion, for example when $\theta = \theta_r$, the optimal water content tends more toward the saturated value, minimizing this source of error. Taking the ratio of D_G^s to D_G^A , the relative diffusion coefficient, D_r (surrogate gas flux), may be expressed in terms of water content as

$$D_r = \eta^{4/3} (1 - \Theta)^{10/3} \quad [7]$$

Equations [5] and [7] can be combined to yield the relative critical gas concentration at the base of the soil, C_r , in terms of media parameters from Eq. [1] as

$$C_r = 1 + \frac{R L^2}{2 C_o D_G^A \eta^{4/3} (1 - \Theta)^{10/3}} \quad [8]$$

Flux (Eq. [2] and [7] as proxy fluxes) and content (Eq. [1] and [8]) of liquids and gases are written in terms of the relative water content and the van Genuchten parameters α and n . An assumption that the processes of liquid and gas transport are adequately described using the SWC is based on information contained in the SWC relating to the media water status (matric head) and air-filled porosity (gas diffusion). In a root environment where water content is either monitored or controlled by tensiometric means, the system operating matric head is an important consideration.

Matric Head Considerations

Maintaining matric head and supplying water within growth media via a porous membrane (stainless steel, plastic, ceramic, etc.) has been demonstrated to be an effective means of controlling the rooting environment both on earth and in a microgravity environment (Morrow et al., 1992, 1993, 1994). Tensiometers, which measure matric head, are also often used to manage irrigation frequency in typical volumetrically controlled systems. In either case, matric head is an important attribute for accurate water control.

For a tension or suction control system, operating matric head plays a critical role in determining not only the media characteristics but also the water supply membrane characteristics (Jones and Or, 1997). For example the working suction of the system should not exceed the bubbling head (function of pore size) of the water supply membrane. If the membrane pore size is decreased, however, there must be a commensurate decrease in membrane saturated hydraulic conductivity to prevent membrane bubbling (i.e., system failure). The media characterization may therefore be partially constrained by the control system characteristics.

The target operating or optimal matric head value, h_o^* (m), should be greater than the bubbling or air-entry head of the matric head control membrane to avoid medium saturation. Porous membrane control systems operated on earth and in microgravity have used values of h_o^* from 0.025 to 0.25 m water column (Wright et al., 1988; Dreschel and Sager, 1989; Koontz et al., 1990; Morrow et al., 1992, 1993). The calculated operating matric head, h_o (m), is found by inverting Eq. [1], giving

$$h_o = \frac{\left(\Theta_o^{n/(1-n)} - 1 \right)^{1/n}}{\alpha} \quad [9]$$

where Θ_o is the optimal water content obtained from the optimization.

The target maximum matric head, h_m^* (m), was selected to allow a range of matric head values greater than h_o^* throughout which water was still present in significant amounts to conduct water to uptake points (i.e., roots and evaporative surfaces). Feddes et al. (1978) suggested that the matric head at which plant growth begins to be limited lies in the range of 0.5 to 1 m of water column, which could serve as a guide for selecting h_m^* where plant stress is undesirable, or larger h if inducing stress is desirable (i.e., reduce stem elongation; Westgate and Boyer, 1985). The calculated maximum matric head, h_m (m), was found by substituting a minimum water content, Θ_{min} , into Eq. [9]. The recommended Θ_{min} value of 0.1 was selected in order to maximize the range of water content while at the same time avoiding the asymptotic portion of the SWC.

Equations [1], [2], [7], and [8] provide expressions of water content, hydraulic conductivity, and O₂ diffusion and concentration as functions of matric head (h), water content (Θ),

media parameters (α and n), container geometry (L), and plant root respiration (R). These parameters were combined with matric head control constraints to form a multiobjective optimization problem.

Optimization of Media Properties

A nonlinear least squares multiobjective optimization problem was cast with an objective function (OF) formulated to maximize liquid and gaseous content and fluxes to plant roots while matching media hydraulic properties to the control system design, given in relative and dimensionless terms as

$$\text{Maximize: } \Theta w_1 + K_r w_2 + D_r w_3 + C_r w_4 \\ - \alpha |h_o - h_o^*| w_5 - \alpha |h_m - h_m^*| w_6 \quad [10]$$

where Θ , K_r , D_r , and C_r are as defined in Eq. [1], [2], [3], and [8] and w_1 through w_6 are individual weighting factors. These weighting factors should, in principle, reflect the relative importance of each of the OF components. The weighting factors should be physically based and consider specific goals, for example, emphasizing the importance of adequate aeration above increased water content or, conversely, deemphasizing dominant terms of the OF. The relative importance of each component of the OF is left for future research and therefore all weighting factors were set equal to 1. The constants h_m^* and h_o^* are the target values for the optimal and maximum matric heads and h_o and h_m are the calculated values (Eq. [9]) for the optimal and maximum matric heads, respectively. The use of relative terms in the OF maintains generality. Constraints of the OF are given as

$$\alpha_{\min} \leq \alpha \\ n_{\min} \leq n \\ \Theta_{\min} \leq \Theta \leq \Theta_{\text{cr}} \\ C_{r \min} \leq C_r \quad [11]$$

where α_{\min} , n_{\min} , Θ_{\min} , and $C_{r \min}$ are the minimum allowable values of α , n , Θ , and C_r , and Θ_{cr} is the critical or maximum allowable Θ . These physically based constraints reflect limitations to parametric values of α and n , which are discussed by van Genuchten and Nielsen (1985). Optimal water content should lie somewhere between the estimated residual or minimum value and some critical value near saturation. Minimum O_2 concentrations should reflect the plant requirements for respiration. The resulting optimized parameters, α and n , provide characteristics of the media.

Determination of Particle-Size Distribution

Models that relate media water retention properties to PSD can potentially provide a means of deriving the PSD from an optimized SWC (Arya and Paris, 1981; Haverkamp and Parlange, 1986; Mishra et al., 1989; Tyler and Wheatcraft, 1989; Rieu and Sposito, 1991; Smettem and Gregory, 1996). The model of Arya and Paris (1981) was inverted in order to scale the optimized SWC (psd) to a PSD. Particle size was determined by minimizing the differences in matric head, h_i , calculated from the Arya and Paris-based capillary rise equation and the optimized SWC (van Genuchten parameters) for the i th particle-size range, given as

$$h_i = \frac{2 \gamma \text{Cos}(\sigma)}{\rho_w g_o r_i} = \frac{\left(\Theta_i^{n/(1-n)} - 1 \right)^{1/n}}{\alpha} \quad [12]$$

where γ (kN m^{-1}), σ , and ρ_w (Mg m^{-3}) are the surface tension,

contact angle, and density of the liquid, respectively, and g_o (m s^{-2}) is the acceleration of gravity. The pore-size radius of the i th particle-size range, r_i (m), is taken from a combination of Eq. [6] and [9] of Arya and Paris (1981), where the void ratio, e , is written in terms of porosity [$e = \eta(1 - \eta)^{-1}$], giving

$$r_i = R_i \left[\frac{2\eta}{3(1 - \eta)} \left(\frac{3w_i}{4\pi R_i^3 \rho_p} \right)^{1-\beta} \right]^{1/2} \quad [13]$$

where R_i (m) is the mean particle radius of the i th particle-size range and ρ_p (Mg m^{-3}) is the particle density. The empirical parameter β (α in Arya and Paris, 1981) is an averaged empirical pore length scaling parameter, which Arya and Paris found to vary from approximately 0.6 up to 1.5 using centimeter-gram-second (cgs) units for the range of soils they considered. In our analysis, we found the value of β to be unit system dependent. Appendix A discusses further insights into its characteristics. The cumulative relative water content, Θ_i , corresponding to each particle-size fraction in Eq. [12] is calculated from the solid mass in the i th particle-size range, W_i (Mg), as

$$\Theta_i = \left(\frac{W_i + W_{i-1}}{2 \sum_{i=1}^N W_i} \right) + \Theta_{i-1} \quad [14]$$

where $0 < \Theta_i < 1$ and is assumed to be directly related to W_i for each particle-size range, N is the total number of ranges, and W_0 and Θ_0 (for $i - 1 = 0$) are equal to 0.

Differences in matric heads calculated from Eq. [12] can be minimized by least squares optimization where the values of W_i are allowed to vary. Particle radius, R_i , could also be a variable in the optimization, but where particle-size ranges are predetermined by sieve size or availability, R_i values are fixed. In the case where R_i is predetermined, β may be initially estimated from Mishra et al. (1989) as

$$\beta = \exp[0.183\sigma_{\ln(2R)}] \quad [15]$$

where $\sigma_{\ln(2R)}$ is the standard deviation of the particle-size cumulative distribution function. This expression for estimating β was found to be satisfactory as an initial guess even though this empirical relation was derived using cgs units. The resulting values of R_i and W_i provided the PSD of the optimal medium. After combining the appropriate mass fractions from each of the respective particle-size ranges, the SWC of the resulting mix was measured and compared with the optimized SWC. If the SWC curves were not well matched, an adjustment of β and a corresponding reoptimization of the R_i and W_i parameters was necessary. The second mixture was again measured and compared with the optimal SWC and generally resulted in a well-matched set of curves.

In summary, van Genuchten (1980) SWC parameters that relate to fluxes and contents of liquids and gases in porous media were optimized and then used to scale the optimized SWC (psd) to PSD by inversion of the Arya and Paris model.

MATERIALS AND METHODS

The optimization routine from a computer spreadsheet (Quattro Pro, Version 6.01, Corel Corp., Ottawa, ON) was used to maximize the OF, Eq. [10] subject to the constraints from Eq. [11]. Constants used in the optimization reflect the plant physiological parameters, media geometry, and water control system design (Table 1). An average respiration rate for root tissue of $10 \mu\text{g O}_2 \text{ mm}^{-3} \text{ d}^{-1}$ was used at a root length density of 0.1 mm mm^{-3} soil and an average root diameter of

Table 1. Values and units of constant, estimated, optimized, and measured parameters from the optimization.

Parameter†	Silica sand	Glass beads	Units
Constant			
ρ_s	2.65	2.46	Mg m ⁻³
R	0.17	0.17	mg O ₂ m ⁻³ s ⁻¹
C_o	233	233	g O ₂ m ⁻³ air
D_o^*	2.3×10^{-5}	2.3×10^{-5}	m ² s ⁻¹
L	0.10	0.10	m
h_o^*	0.2	0.8	m
h_m^*	1.0	1.4	m
Estimated			
α	2.5	1.2	m ⁻¹
α_{min}	0.001	0.001	m ⁻¹
n	2.5	7.5	
n_{min}	1.2	1.2	
Θ	0.5	0.5	
Θ_{min}	0.1	0.1	
Θ_{cr}	0.85	0.85	
η	0.44	0.35	m ³ m ⁻³
θ_s	0.40	0.32	m ³ m ⁻³
θ_r	0.05	0.05	m ³ m ⁻³
C_r	0.025	0.025	g O ₂ m ⁻³ air
K_s	5.0×10^{-4}	1.0×10^{-4}	m s ⁻¹
Optimized			
α	3.43	1.04	m ⁻¹
n	2.85	6.99	
Θ_o	0.83	0.81	
Measured			
η	0.40	0.39	m ³ m ⁻³
θ_s	0.36	0.35	m ³ m ⁻³
θ_r	0.03	0.05	m ³ m ⁻³
K_s	4.6×10^{-4}	6.0×10^{-5}	m s ⁻¹

† Parameter definitions are given in Appendix C.

0.1 mm, giving $R = 0.17 \text{ mg O}_2 \text{ m}^{-3} \text{ s}^{-1}$ (De Willigen and Van Noordwijk, 1987). Values of D_o^* and C_o used were calculated assuming temperature of 25°C and 85 kPa. The value of L used was 0.1 m, a media depth used in previous plant growth studies in microgravity (Ivanova et al., 1993; Bingham et al., 1996b). Selected target operating and maximum matric head values for sand were similar to head values previously used in suction-controlled systems on earth and in microgravity. Target values for glass beads were selected to test the theory both with a narrower PSD and using smaller particles (more negative heads).

Silica sand (Unimin Corp., Emmitt, ID; Wisco Inc., Brigham City, UT) was sieved to 10 size fractions ranging from 38 to 2000 μm diameter (see Table 2). Glass beads (Cataphote, Inc., Jackson, MS) of 63 to 125 μm were also tested. Homogenization of the mixture was critical to successfully matching the predicted SWC curve. The sand or glass bead mixture was deposited by laying down 2-mm layers and compacting (Olivera et al., 1996) into 500-mL Büchner-type funnels having medium fritted glass disks. A hanging water column was used to determine the SWC (Klute, 1986). Saturated hydraulic conductivity was determined using a constant-head method (Klute and Dirksen, 1986). Porosity was estimated from known particle density and an initial estimate of bulk density. Alternatively, η may be estimated based on binary mixing models as discussed in Appendix B.

RESULTS AND DISCUSSION

Optimized Media Parameters

The optimal media parameters (α and n) provide the necessary information for synthesis of the optimal growth medium, whereas the optimal water content (Θ_o)

Table 2. Media particle-diameter ranges for glass beads and silica sand used in media synthesis.

Glass beads	Sand
μm	
63–53	38–53
74–63	53–104
88–74	104–180
105–88	180–250
125–105	250–295
149–125	295–500
	500–589
	589–840
	840–1000
	1000–2000

indicates the operating point or moisture level at which fluxes and contents are maximized. The optimized values of α , n , and Θ_o are given in Table 1 for sand (38–2000 μm) and glass beads (63–125 μm). The effect of varying α and n on the OF surface is illustrated by the contour plot of Fig. 2, where the distinct peak gives an indication of the significance of parameter optimality and of maximizing gas and liquid flux and content, the OF. Reduction of α (smaller pores) or n (wider psd) produces a steep reduction in the OF surface caused by the exponentially increasing deviation (e.g., $h_i \propto r_i^{-1}$) from h_o^* and h_m^* . The matric head constraints used in the OF have the largest impact on the optimization results. Removal of the two matric head constraints from the OF (Eq. [10]) resulted in values, independent of α , of 65 to 82% of the peak in Fig. 2 for n values from 2 to 7, respectively.

Estimated values shown in Table 1 were used in the initial iteration of the optimization and eventually became either optimized or measured values. From our work, it appears that initial estimates of α , n , and Θ only slightly perturb the final solution within a range (not well defined) around the optimal values, but may lead to unstable solutions for initial estimates deviating greatly from the optimal values. Some iteration of initial estimates may be required for gaining confidence in solution optimality.

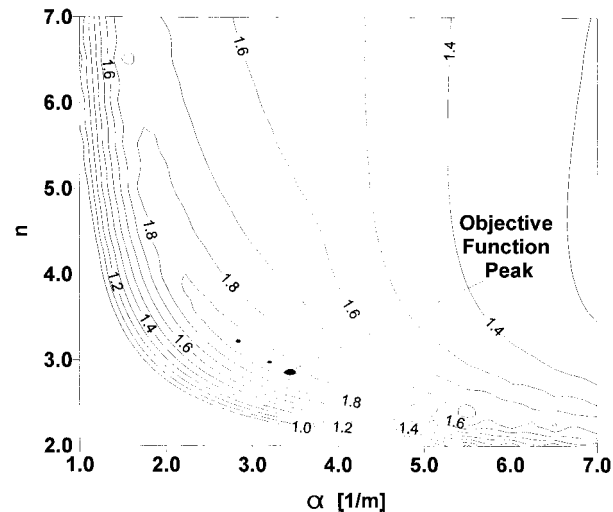


Fig. 2. Objective function (OF) surface in the α - n parameter space at the optimal relative water content of 0.83 for sand.

Optimization Considerations

The relative matric head (h_r) plotted in Fig. 3 matches precisely with h_o^* at Θ_o and with h_m^* at the assumed minimum water content, Θ_{min} . Thus the matric head constraints largely control the psd (n) and bubbling head (α) of the medium and therefore the media parameter optimality is largely dependent on the models and constraints forming the OF. Without matric head constraints, the optimization gives unrealistically large values of both α and n , indicating a medium with very large, single pores and having a near-horizontal SWC. This scenario produces large changes in water content (easily saturated) with small changes in matric head, requiring greater accuracy in a water control system. The dilemma of maximizing both liquid and gas fluxes simultaneously is illustrated by the inverse relation of liquid conductivity (K_r) and gaseous diffusion (D_r) as functions of Θ . The rapid decrease in relative O_2 content (C_r) between 0.8 and 0.9 Θ imposes an upper boundary for finding Θ_o . Increasing either L or R in Eq. [8] shifts this boundary to the left, effectively reducing Θ_o . Maintaining such high water contents, uniformly, in earth's gravity, is unlikely (function of psd and media depth), while in microgravity both higher sustained water contents and more uniform distributions have been measured in coarse-sand-size media (Bingham et al., 1996a).

Scaling Pore Size to Particle Size

The core of the proposed methodology combines the optimized SWC with the inverted Arya and Paris model to synthesize a PSD from the optimal psd. The initial estimate of β (1.22, see Appendix A) was determined from Mishra et al. (1989), and a sand medium was constructed according to the resulting PSD. The measured SWC was compared with the optimized SWC, revealing a considerable overestimate of β , which effectively overscaled the sand pore sizes. The initial estimate of β for glass beads (1.06) turned out to be very near the

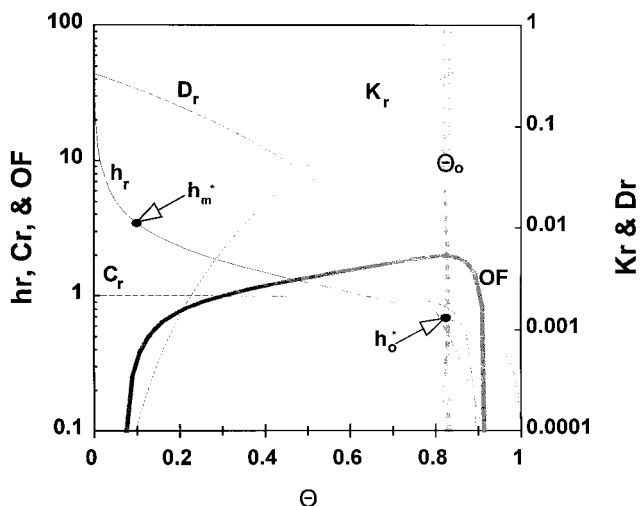


Fig. 3. Optimization results showing the objective function (OF), with relative matric head (h_r), unsaturated hydraulic conductivity (K_r), O_2 diffusion (D_r), and O_2 content (C_r) as functions of relative water content (Θ). The optimal water content occurs at the OF peak.

value fitted from the first iteration. By fitting the Arya and Paris model to the measured SWC, new β values of 1.08 and 1.05 (1.16 and 1.09 using cgs units) were determined for sand and glass beads, respectively. A second determination of PSD was carried out, followed by measurement and comparison of the SWC for the second iteration (Fig. 1). Histograms of particle sizes obtained from the first and second estimates of β are shown in Fig. 4a for sand and Fig. 4b for glass beads. In each case, particle-size fractional content shifted to the smaller particle-size ranges to compensate for overestimation of β . A good match was generally found after one or two iterations.

Comparison of Optimized vs. Measured SWC

The optimized SWC (described by α and n) and replicated measurements of the SWC for sand are plotted in Fig. 5a. The measured SWC fits the optimized SWC very closely after two iterations of the scaling parameter β . The resulting sand mixture exhibits optimal characteristics described by the optimized parameters. For glass beads (Fig. 5b), the measured SWC exhibits a

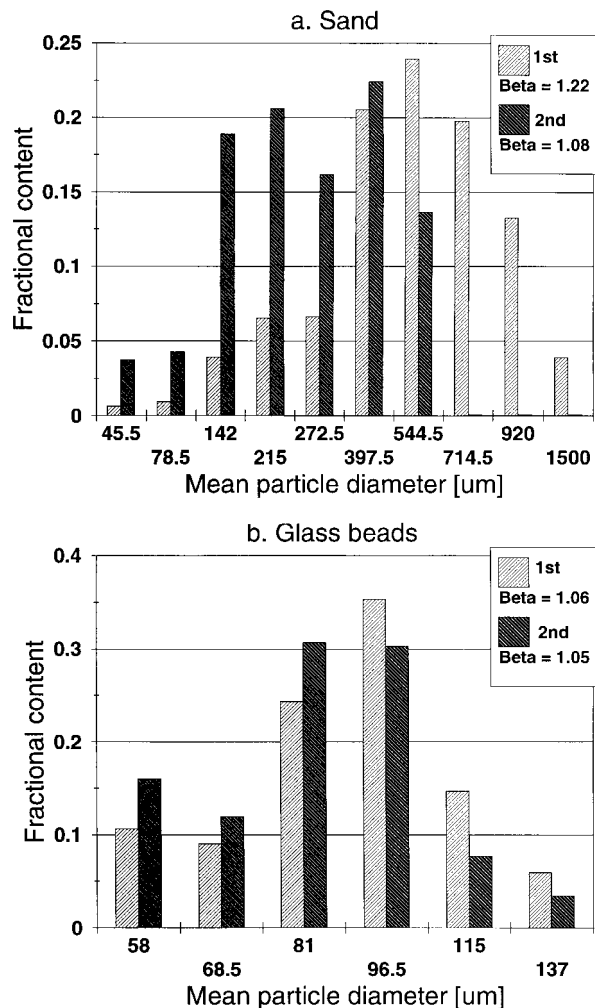


Fig. 4. Particle-size histogram for (a) sand and (b) glass bead mixtures obtained from the first and second estimates of the pore scaling parameter β .

narrower psd than the optimized SWC despite a best-fit value of β . Increasing the total glass bead size ranges to 10 (40–194 μm) and again to 15 (13–328 μm) did not improve the observed disparity between measured and optimized SWC curves. Figure 5b reveals that the larger glass bead sizes were overscaled (i.e., smaller β required) and finer sizes were underscaled. This phenomenon is not clearly understood but may be affected by the narrower PSD. Despite the inability to exactly match the optimized SWC using glass beads, differences between measured and optimized SWC lie within the expected variation in SWC for soils.

SUMMARY AND CONCLUSIONS

We developed a new method for designing porous media characteristics by maximizing the dynamic availability of liquids and gases to plant roots. Plant physiological requirements, media depth, and target matric heads served as constraints for a multiobjective optimization problem with media parameters as variables. The optimization could also incorporate other physiological or physical models not presented here. Media PSD was determined by iteratively adjusting the pore-size scaling parameter to fit the SWC described by the optimized media parameters. After one or two iterations, the measured SWC of the synthesized media (sand) was in good agreement with the optimized SWC, using a wide range of particle sizes. Application to a narrow range of glass bead sizes revealed an apparent limitation of the Arya

and Paris (1981) model to adequately scale psd to PSD using distributions spanning less than an order of magnitude. The methodology is therefore limited only by the models selected, a key component being the ability to correctly scale psd to PSD. The outlined procedure demonstrates the ability to design and synthesize porous media to maximize fluxes of liquids and gases to plant roots. The concept of media selection based on optimizing media properties should lend itself to other applications where psd and PSD are adequately described by physical models.

APPENDIX A

Properties of the Arya & Paris β Parameter

The following discussion of the pore length scaling parameter, β , provides additional information on its definition and role as a scaling parameter of particle to pore size (matric head). The choice of the unit system or scale and its impact on β values and consequently pore to particle scaling are presented. We distinguish β , the averaged pore scaling parameter discussed here, from β_i , the individual pore scaling parameter of the i th particle-size range, which can be written in terms of the particle radius and matric head (measurable parameters), using Eq. [14] and substituting from Eq. [12], as

$$\beta_i = 1 - \frac{\ln\left(\frac{3}{2} \frac{1 - \eta}{\eta} \left[\frac{2 \gamma \text{Cos}(\sigma)}{\rho_w g_o h_i R_i} \right]^2\right)}{\ln\left(\frac{3W_i}{4\pi \rho_p R_i^3}\right)} \quad [16]$$

Since β_i is a unitless parameter, the fact that its calculated value is sensitive to selection of the scale or unit system is not intuitive and calls for further discussion. Arya and Paris (1981, 1982) and most subsequent literature comparing values of the scaling parameter (Schuh et al., 1988; Mishra et al., 1989; Tyler and Wheatcraft, 1989) have used the centimeter–gram–second (cgs) system of units; however, Jonasson (1992) evidently used a variety of units (e.g., millimeter, meter, gram, kilogram) and we used meter–kilogram–second (mks) units. We noted that values of β_i computed using cgs units were not reproducible using the mks system. The scale dependency is attributable to the requirement that all W_i sum to unity and therefore values of W_i remain constant for any given set of units. For example, the denominator of Eq. [16] increases sixfold when units are changed from cgs to mks, due to the R_i^3 term, resulting in a different value of β_i . With regard to the mks system, it is necessary to use mass units of megagram instead of kilogram since the summation of all W_i must equal one mass unit (i.e., gram or megagram) and particle density combines length and mass scales (e.g., 2.65 g cm^{-3} or Mg m^{-3}). The conversion of β_i from one unit system to another is accomplished by adjusting the units in Eq. [16] for a given set of data. It appears that conversion of β to a different set of units is more complex since its value is based on the weighted effect of all particle-size ranges.

Since particle radius and matric head dominate the dependence of β_i , its surface was plotted in Fig. 6 as a function of these two variables using Eq. [16]. Note that the surface of β_i for larger particle radii (1000 μm) and lower matric heads (0.02 m) is ill defined in the cgs system, compared with the mks system, which is stable well beyond the window of interest shown. To further illustrate the effect of different systems of units on β_i , we reference Arya and Paris (1982; Table 2) and computed β_i using mass units of 1 mg, 1 g, and 1 Mg with

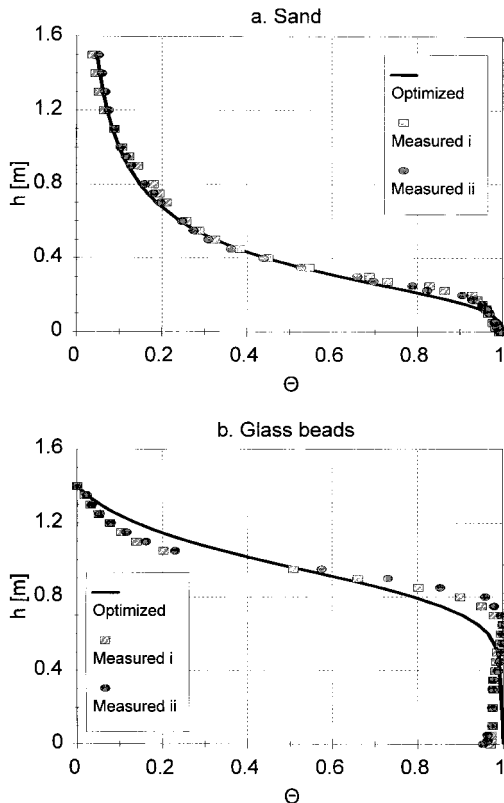


Fig. 5. Comparison of optimized and measured substrate–water characteristic for (a) sand and (b) glass beads, where h is matric head and Θ is the relative water content.

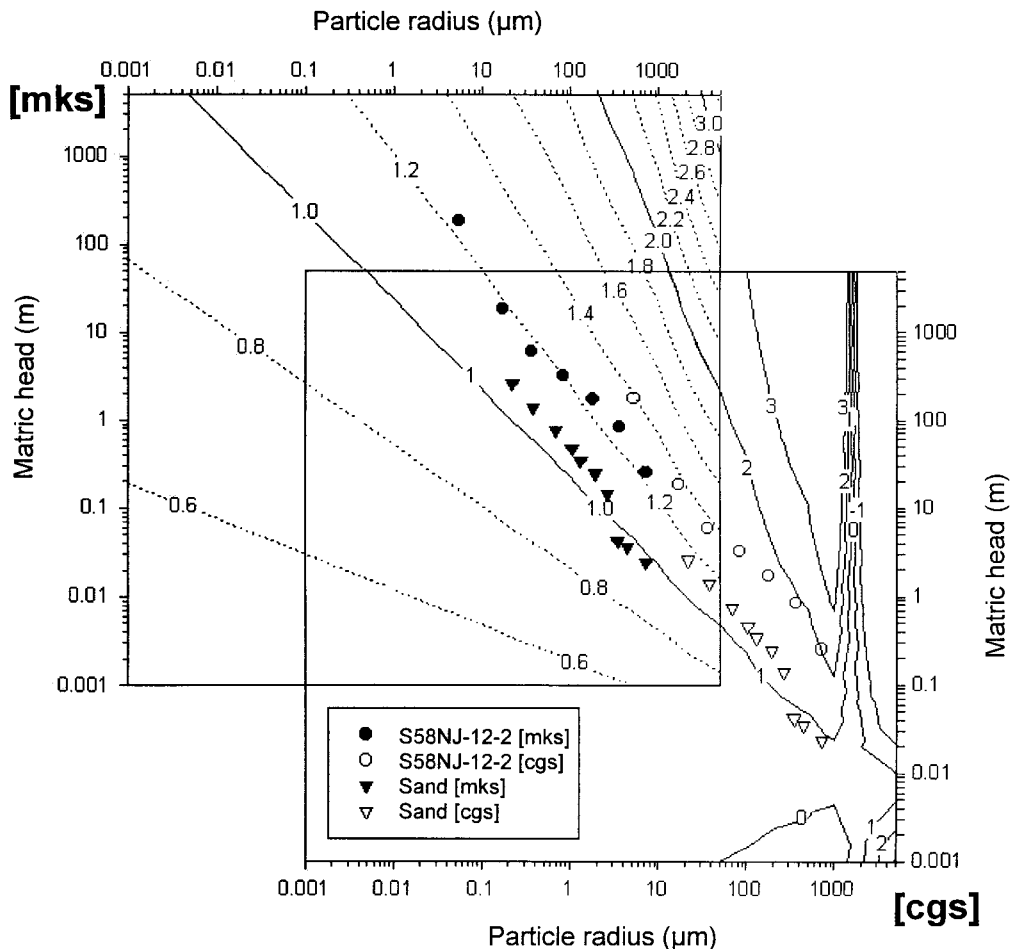


Fig. 6. Surface of the pore scaling parameter, β , as a function of particle radius and matric head. Windows indicate two different unit scales: centimeter-gram-second (cgs) and meter-kilogram-second (mks).

corresponding length units of millimeter, centimeter, and meter, respectively. For their particle radius of $37.5 \mu\text{m}$ and the corresponding matric head of 6.28 m and using their other values as presented, the calculated pore scaling parameters from Eq. [16] are 1.89, 1.38, and 1.18, respectively.

Using our measured data for sand and the New Jersey soil S58NJ-12-2, horizon B23t (Soil Conservation Service, 1974), referenced by Arya and Paris (1982), values of β_i were calculated and plotted on the surface in Fig. 6 using both cgs and mks systems of units. For easier observation of how the window of interest shifts from one unit system to another, units of the axis for each window are consistent. Moving from the cgs to the mks unit system, the window of interest shifts two orders of magnitude upward and to the left, which results in a shift in the plotted data parallel to a β value of 1. This shift results in reduced β values for larger unit scales, due to the diverging nature of the surface moving parallel to and above $\beta = 1$. It is therefore imperative to identify the unit system used either when calculating values of β_i , or when assuming β to estimate matric head from particle-size distribution data. The value of β for sand (1.16 in cgs units) was smaller than weighted and arithmetic mean values of β_i (1.37 and 20.7) but was closer (1.18 and 1.17, respectively) when the three outliers in Fig. 6 were removed. For the New Jersey soil, the β value (1.39) was also lower than the weighted and arithmetic mean values (1.53 and 1.96) and elimination of the lowest two points (associated with large values of β_i) also improved estimates (1.46 and 1.52). In the mks system, either method of averaging

produced almost identical values of β in both the case of sand and the New Jersey soil, with no outlier removal.

For $\beta = 1$, Eq. [14] reduces to a function of the porosity given as

$$r_i = R_i \left(\frac{2}{3} \frac{\eta}{1 - \eta} \right)^{0.5} \tag{17}$$

Cubic, orthorhombic, and tetrahedral packing arrangements of uniform size spheres exhibit pore radii of 0.73, 0.53, and 0.41 times the sphere radii for their associated porosities of 0.48, 0.40, and 0.26, respectively (Gupta and Larson, 1979). Equation [17] produces slightly larger pore radii, giving particle radii multipliers (square root term) of 0.79, 0.66, and 0.48 for the three porosities mentioned. This comparison indicates that the pore sizes calculated with the Arya and Paris model are slightly oversized, and therefore, as stated by Arya and Paris (1981), one should always expect β to be >1 (e.g., glass beads = 1.05). The three data points from sand in Fig. 6 that plot below $\beta = 1$ are low due to their small mass contribution ($W_i = 0.001$), which scales them to matric heads below the bubbling head of the medium as Θ approaches a value of 1 (see Fig. 4). Also, because of the dependence of β_i on porosity, we compared contour plots of β for porosities of 0.36 and 0.60 but noted only a slight perturbation between the two surfaces.

A final observation from the data plotted in Fig. 6 relates to the vertical shift in matric head, for any given particle size, associated with the inclusion of fines in the New Jersey soil

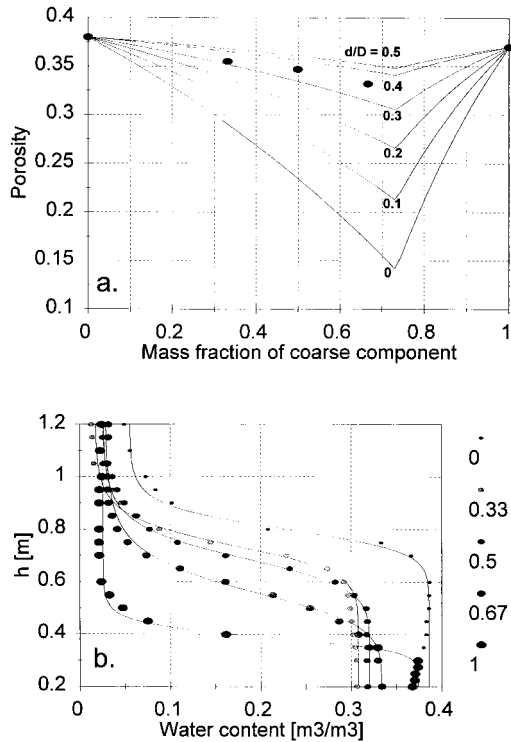


Fig. 7. (a) Substrate–water characteristic curves for mixtures of glass bead sizes of 100 and 200 μm of different mass fractional contents of the coarse (200 μm) component (d/D) and (b) estimated porosity as a function of the mass fraction of the coarse component, D , of binary mixtures whose diameter ratios, d/D , vary from 0 to 0.5. Data points are measurements of porosity for the glass bead mixtures; h is matric head.

(17, 55, and 28% sand, silt, and clay, respectively) compared with the sand mixture, which contains relatively no silt or clay. The shift to higher matric head for a same-size particle probably results from the reduction in overall pore size due to the presence of the silt and clay fractions leaving pores smaller than those formed without the contribution of the finer material (Wu and Vomocil, 1992). Thus, larger values of β may partially result from the presence of finer material, which is often only associated with the smallest particle fraction, a fraction whose contribution is half that of intermediate size fractions in the Arya and Paris analysis. Additional theoretical limitations of the Arya and Paris analysis were detailed by Schuh et al. (1988).

APPENDIX B

Estimating Porosity and Saturated Hydraulic Conductivity

Uniform-sized particles form a near-ideal system for portraying the effects of particle mixing on porosity and estimating saturated conductivity. Here we seek to provide an independent means of estimating porosity and saturated conductivity for the optimization, either as an initial guess or by incorporating η and K_s directly into the optimization where absolute rather than relative values are of interest. We start with binary mixtures of 100- and 200- μm particles whose SWCs were measured and plotted in Fig. 7a. Increasing the fraction of the fine component not only causes a decrease in the overall matric head, h , but also alters the porosity of the mixture as indicated by the saturated water content values ($h = 0.2$ m). The decrease in head is associated with the

reduction in pore size due to the finer particles partially filling some of the large pores, a phenomenon that also accounts for reduced porosity. The net effect is to reduce the overall size of pores and thus increase the matric head associated with all particle-size ranges as seen by comparing sand with the New Jersey soil in Fig. 6. The quality of the mixture thus influences the Arya & Paris pore-scaling parameter β .

The binary approximation for particle systems can be useful for predicting porosities of particle mixtures and is influenced by the fractional contribution of each component as well as by the diameter ratio of the two sizes. Furnas (1931) presented a methodology for estimating mixture porosities of two, three, and four components where individual porosities of each component are the same. He derived an empirical expression that predicts the reduction in porosity as a function of the diameter ratio of components. More recently, Koltermann and Gorelick (1995) presented a fractional packing model that corrects for the “ideal” model’s underestimation of porosity by measuring the minimum achievable porosity of a mixture. Their model accounts for differing individual component porosities. While a detailed discussion of the models is beyond the scope of this study, we feel that identifying the usefulness of combining these theories potentially adds to the power of the optimization and further explains the particle–pore relationships discussed above.

The measured minimum porosity requirement in the model of Koltermann and Gorelick (1995) was replaced by the empirical relation of Furnas (1931), which includes consideration of the component diameter ratio assuming minimum theoretical packing for ratios approaching zero. In Fig. 7b, the combined model is plotted using measured porosities from 100- (d) and 200- μm (D) glass beads for the different diameter ratios shown. Measured porosities for coarse component mixtures of 0.33, 0.5, and 0.67 are slightly overestimated by the model ($d/D = 0.5$) with both corresponding to saturated water contents shown in Fig. 7a.

To illustrate its application to estimating porosity, prior to any optimization we take a range of sieve-separable particle sizes (38–2000 μm) and assume a normal distribution giving values for D_{25} (grain diameter for which 25% of material is finer) and D_{75} of 590 and 1400 μm , respectively, and measure the porosity of the material of interest (i.e., porosity of sand = 0.42). Applying the combined models of Koltermann and Gorelick (1995) and Furnas (1931) gives an estimated mixture porosity of 0.4 for $d/D = 0.43$. For comparison, we also took D_{25} and D_{75} from the measured PSD curves of sand and the New Jersey soil, giving diameter ratios of 0.4 and 0.08, respectively. Measuring coarse- and fine-component porosities of 0.46 and 0.43 for sand and assuming 0.4 and 0.6 for the New Jersey soil, the estimated mixture porosities for the sand and soil are 0.41 and 0.32, compared with measured mixture porosities of 0.4 and 0.36, respectively.

From the estimate of porosity and mean particle diameter, one can use an expression for saturated conductivity such as Kozeny–Carman (Bear, 1972):

$$K_s = \left(\frac{\rho_w g_0}{\mu} \right) \frac{d_m^2 \eta^3}{180(1 - \eta)^2} \quad [18]$$

where μ is dynamic viscosity. The mean grain diameter, d_m (m), is calculated from either the geometric or harmonic mean of d and D as described by Koltermann and Gorelick (1995). For the initial estimate of porosity for sand using both geometric and harmonic mean diameters, we calculate K_s of 8.6×10^{-5} and 7.2×10^{-5} m s⁻¹, respectively, where the measured K_s was 4.6×10^{-4} m s⁻¹. Using the optimized sand PSD, the geometric and harmonic mean diameters produce K_s of $1.0 \times$

10^{-5} and $8.4 \times 10^{-6} \text{ m s}^{-1}$, respectively. The New Jersey soil has a reported K_s of $7.1 \times 10^{-8} \text{ m s}^{-1}$ and using Eq. [18] with geometric and harmonic means, the calculated K_s is 6.6×10^{-9} and $1.7 \times 10^{-9} \text{ m s}^{-1}$, respectively. This method of estimating K_s produces estimates generally within one order of magnitude (Koltermann and Gorelick, 1995), with the geometric mean producing closer estimates for the examples cited.

In summary, binary mixing models provide a limited, though useful means of estimating mixture porosity and saturated conductivity and such models may potentially be incorporated into the optimization itself at the cost of adding to the complexity of the optimization.

APPENDIX C

Symbols

C_G	gas concentration, g m^{-3}
C_o	atmospheric gas concentration, g m^{-3}
C_r	relative gas concentration
$C_{r \text{ min}}$	minimum allowable relative gas concentration
D	mean diameter of large component of binary mixture, m
D_G^A	air-gas diffusion coefficient, $\text{m}^2 \text{ s}^{-1}$
D_G^S	soil-gas diffusion coefficient, $\text{m}^2 \text{ s}^{-1}$
D_r	relative diffusion coefficient
D_{25}	grain diameter for which 25% of material is finer
D_{75}	grain diameter for which 75% of material is finer
d	mean diameter of small component of binary mixture, m
d_m	mean grain diameter of particle mixture, m
e	void ratio
g_o	acceleration due to gravity, m s^{-2}
h	matric head, m
h_i	matric head of the i th particle-size range, m
h_m	computed maximum matric head, m
h_m^*	target maximum matric head, m
h_o	computed operating matric head, m
h_o^*	target operating or optimal matric head, m
h_r	relative matric head
K	hydraulic conductivity, m s^{-1}
K_r	relative hydraulic conductivity
K_s	saturated hydraulic conductivity, m s^{-1}
L	depth of growth medium, m
N	total number of particle-size ranges
n	empirical parameter related to the pore-size distribution
n_{min}	minimum allowable value for n
OF	objective function
PSD	particle-size distribution
psd	pore-size distribution
R	respiration rate per unit volume, $\text{g m}^{-3} \text{ s}^{-1}$
R_i	particle radius in the i th particle-size range, m
r_i	pore radius in the i th particle-size range, m
SWC	substrate-water characteristic
t	time, s
W_i	solid mass fraction in the i th particle-size range, Mg
w_1, \dots, w_6	weighting factors for components of the objective function
x	distance, m
α	empirical parameter inversely related to the bubbling pressure, m^{-1}
α_{min}	minimum allowable value for α , m^{-1}
β	pore scaling parameter
β_i	pore scaling parameter of the i th particle-size range
γ	liquid surface tension, kN m^{-1}
η	total porosity, $\text{m}^3 \text{ m}^{-3}$

μ	dynamic viscosity, Pa s
Θ	relative water content
Θ_{cr}	critical or maximum allowable relative water content
Θ_i	relative water content of the i th particle-size range
Θ_{min}	minimum allowable relative water content
Θ_o	optimal relative water content
θ	absolute water content, $\text{m}^3 \text{ m}^{-3}$
θ_r	residual water content, $\text{m}^3 \text{ m}^{-3}$
θ_s	saturated water content, $\text{m}^3 \text{ m}^{-3}$
ρ_p	particle density, Mg m^{-3}
ρ_w	liquid density, Mg m^{-3}
σ	liquid contact angle
$\sigma_{\ln(2R)}$	standard deviation of the particle-size cumulative distribution function
ϕ	air-filled porosity, $\text{m}^3 \text{ m}^{-3}$

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