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Hydrology of Horticultural Substrates: I. Mathematical Models for Moisture Characteristics of Horticultural Container Media

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Abstract. **Moisture retention data were collected for five porous materials: soil, phenolic foam, and three combinations of commonly used media components. Two mathematical functions were evaluated for their ability to describe the water content–soil moisture relationship. A cubic polynomial function with linear parameters previously used on container media was compared to a closed-form nonlinear parameter model developed to describe water conductivity in mineral soils. In most tests for precision, adequacy, accuracy, and validation, the nonlinear function was superior to the simpler power series. The nonlinear function provides an excellent tool for describing the water content for media with widely varying physical properties.**

Understanding the physical environment surrounding roots in containers (relative volumes of air, water, and solid) is based on the relationship between water energy status and water content of the medium. This relationship is a reflection of the pore size distribution of the medium. A plot of this relationship, i.e., a plot of volumetric wetness (Θ) vs. soil water pressure (negative quantity) or soil moisture tension (MT, positive quantity) is called the soil moisture characteristic or moisture retention curve (4).

Ever since Bunt (3) first reported moisture retention curves for pot-plant media, there has been considerable effort to determine the utility of these curves in explaining plant growth, and the best way to quantify these data for both descriptive and predictive purposes. White (20) realized the importance of moisture retention curves on water content in containers and introduced the concept of "container capacity" (in contrast to field capacity).

Fonteno et al. (7) used the classification suggested by De Boodt and Verdonck (6) and introduced regression analysis to describe the moisture retention curve for horticultural media. A linear relationship between Θ and moisture tension was found between 0 and 2 kPa, whereas a quadratic relationship existed from 2 to 10 kPa. Several researchers developed a cubic regression model to describe the moisture retention curve, with the goal of predicting the container-specific values of air space and container capacity (8, 10, 16).

Soil scientists have also had great interest in using moisture retention models (5). As reviewed by Van Genuchten and Nielson (18), there are at least four basic nonlinear empirical functions relating Θ to MT that are continuously differentiable (smooth): King (11), Laliberte (12), Su and Brooks (15) and Van Genuchten (17). The Van Genuchten model (17) is gaining acceptance in the field of soil science.

Van Genuchten's function stems from an analysis by Brooks and Corey (2), given by

$$\Theta = (\Theta_s - \Theta_r)(\alpha h)^L + \Theta_r \qquad [1]$$

where Θ_s is the saturated water content, Θ_r is the residual water content, α is the inverse of the "air entry value", h is the log of the moisture tension, and L is the "pore size distribution index". In order to provide a better fit, Van Genuchten (17) proposed:

$$\Theta = \Theta_r + (\Theta_s - \Theta_r)/[1 + (\alpha h)^n]^m \qquad [2]$$

where he assumed unique relations between n and m, i.e., $m = 1 - (1/n)$. To improve flexibility of the model, the "new" model (18) has removed this restriction on n and m, so all five parameters are independent. Θ_s and Θ_r are known empirical parameters, while α, n, and m are unknown and are determined using standard nonlinear least squares parameter estimation methods.

Quantifying the soil profile (or container) air and water variables is important not just in specific applications, such as the container work of Karlovich and Fonteno (10) or the unsaturated conductivity modeling of Van Genuchten and Nielsen (18), it is also necessary in developing overall growth models for containerized crops, whether they are evapotranspiration models, transpiration-available water models, or transpiration-Θ models (9, 13, 19).

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Because container media used in horticulture have widely varying physical properties as compared to field soils, and because two recent methods used to describe each vary considerably [Karlovich and Fonteno (10) vs. Van Genuchten and Nielsen (18)], research was initiated to evaluate these two mathematical models using data collected on soil-based, soilless, and synthetic container media commonly used in horticultural growing systems.

Materials and Methods

Eight replications of four media (Table 1) were packed in 347.5-ml cylindrical aluminum rings (7.6 cm in diameter, 7.6 cm in height) using modified procedures of Bilderback et al. (1). Three rings were stacked vertically, filled with a medium and tapped against a laboratory table from a height of ≈10 cm sufficient times to obtain certain bulk densities in the middle ring (Table 1). The other two rings were discarded. The bulk densities were chosen to be representative of the bulk densities found in containers under commercial production practices. The media were: 1—Cecil clay loam; 2—1 peat : 1 vermiculite (v/v), similar to many of the so-called "peat-lite" mixes; 3—3 pinebark : 1 peat : 1 sand (by volume); and 4—1 Wagram sandy loam soil : 1 peat : 1 sand (by volume); 5—synthetic phenolic foam material (Oasis Root Cube; Smithers Oasis Co., Kent, Ohio). Because of its basically solid nature, the foam material was prepared using an aluminum cutter ring (7.6 cm in diameter, 2.5 cm in height) placed atop the above-mentioned ring and hand-pressed into air-dried foam blocks (23.0 × 10.8 × 7.9 cm). No compression or other alteration of the foam material was observed.

All rings were seated onto the porous plate of a Kimax 600 ml 90 F Buchner filter funnel and saturated with water by slowly adding water between the funnel wall and the outside of the aluminum ring (7) over 24 to 48 hr. An airtight lid was placed on top of the funnel and positive air pressures were applied in increments that resulted in pressures at the medium center of 3.8, 10, 20, 40, 50, 75, 100, 200, 300 cm (H_2O). Volume outflow was recorded for each increment. Normally, a period of 48 hr was required to establish equilibrium at pressures <50 cm and 24 hr for higher pressures. After measurement at 300 cm, each sample was removed and oven dry bulk density determined by calculating the volume of each sample and weighing each sample after drying 24 hr at 105°C (10).

Volume outflow was converted to percent volumes and were regressed against the log of the moisture tension values converted to kiloPascals. The MT values were transformed by adding the integer 1 to each. Thus, the log of the transformed MT

Table 1. Description of growing substrates.

Medium No.	Medium Description	Bulk density ($g \cdot cm^{-3}$)	Maximum particle diam (cm)
1	Cecil clay loam	0.999	0.200
2	1 peat[z] : 1 vermiculite[y]	0.151	0.635 : 0.635
3	3 bark[x] : 1 peat : 1 sand[w]	0.408	1.270 : 0.200
4	1 soil[v] : 1 peat : 1 sand	1.107	0.200 : 0.200 : 0.635
5	Phenolic foam[u]	0.011	Matrix

[z]Canadian sphagnum peat.
[y]Horticultural vermiculite #2.
[x]Pine bark humus.
[w]Builder's grade sand.
[v]Wagram sandy loam.
[u]Oasis Rootcube (Smithers Oasis Co., Kent, Ohio).

data is greater than or equal to zero. The data were described by two models, the cubic polynomial (power series) [as discussed by Karlovich and Fonteno (10)] and the nonlinear equation [developed van Van Genuchten and Nielsen (18)].

The cubic polynomial (Model I) is given by

$$Y = a + bX + cX^2 + dX^3 \quad [3]$$

with X = log [(kPa of moisture tension·9.8) + 1], and parameters a, b, c, and d being unknown.

The nonlinear model (Model II) is defined as

$$\Theta = \Theta_r + (\Theta_a - \Theta_r)/[1+(\alpha h)^n]^m \quad [4]$$

where Θ_s is the mean percent moisture at saturation, Θ_r is the mean percent moisture at asymptotic residual, and α, n, and m are unknown. Estimation of parameters α, n, and m is aided using their partial derivatives:

$$\alpha = (\Theta_s - \Theta_r)\cdot m\cdot\{1/[1 + (\alpha\cdot X)^n]\}^{(m-1)}\cdot \{-1[1 + (\alpha\cdot X)^n]^2\}\cdot n\cdot X^n\cdot\alpha^{(n-1)} \quad [5]$$

If X = 0 then the derivative of n = 0, otherwise

$$n = (\Theta_s - \Theta_r)\cdot m\cdot\left[\{1/[1+(\alpha\cdot X)^n]\}^{(m-1)}\right]\cdot \{-1/[1+(\alpha\cdot X)^n]^2\}\cdot(\alpha\cdot X)^n\cdot \mathrm{Ln}(\alpha\cdot X) \quad [6]$$

and

$$m = -(\Theta_s - \Theta_r)\cdot \{1/[1+(\alpha\cdot X)^n]\}^m\cdot \mathrm{Ln}[1 + (\alpha\cdot X)^n]. \quad [7]$$

Van Genuchten suggested that Θ_r can be calculated along with α, n and m. However, Stephens and Rehfeldt demonstrated improved model accuracy using an empirical Θ_r (14). We therefore included Θ^r as a measured parameter.

Various statistical tests were used to evaluate the significance, precision, adequacy, and assumptions of the two models. Model accuracy (validity) was determined by comparison of predicted to measure data.

Results and Discussion

Both models for all five media were significant based on the F test in analysis of variance (data not shown). These results only indicate that variation due to regression was significantly greater than the residual variation.

Comparison of predicted curves to observed data gives some insight into model adequacy. For the Cecil clay loam, the distinction between the two models is not great (Fig. 1), and both were considered good predictive tools. The polynomial was unable to predict means for the peat and bark based mixtures (media 2 and 3, respectively). However, it provided a basic understanding of the relationships (Figs. 2 and 3). The soil-based mixture (medium 4, Fig. 4) illustrated a type of failure of the polynomial often seen in poorly drained media in related studies, where, at very low MT, the predicted moisture values rose above saturation, with the opposite effect near the dry end of the curve. This type of failure is more obvious for the phenolic foam (medium 5, Fig. 5), where the polynomial predictions were off-scale at both ends of the curve. In this situation, the polynomial failed both as a tool for prediction and in providing a basic understanding of the relationship.

Regression precision was evaluated using the regression coefficient SE, the mean square error, and the coefficient of deter-

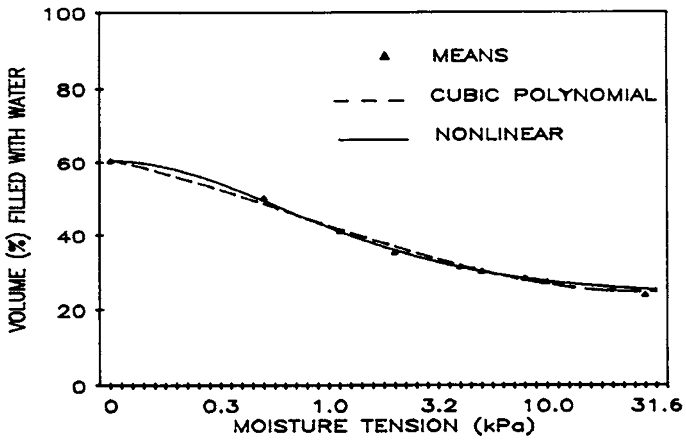

Fig. 1. Means and predicted moisture retention curves for cubic polynomial (Model I) and nonlinear (Model II) regression for medium 1 (Cecil clay-loam).

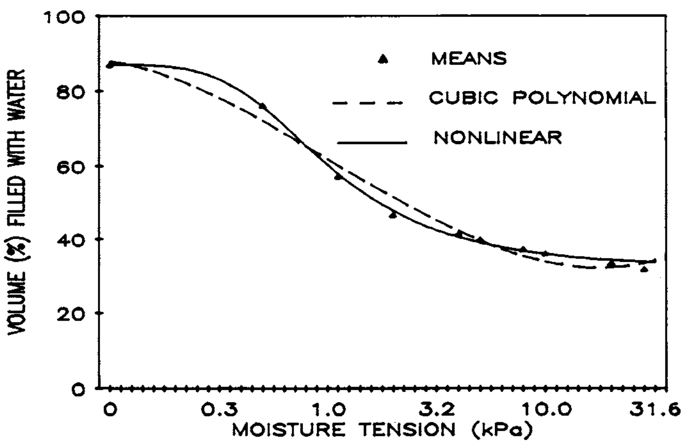

Fig. 2. Means and predicted moisture retention curves for cubic polynomial (Model I) and nonlinear (Model II) regression for medium 2 (1 peat : 1 vermiculite).

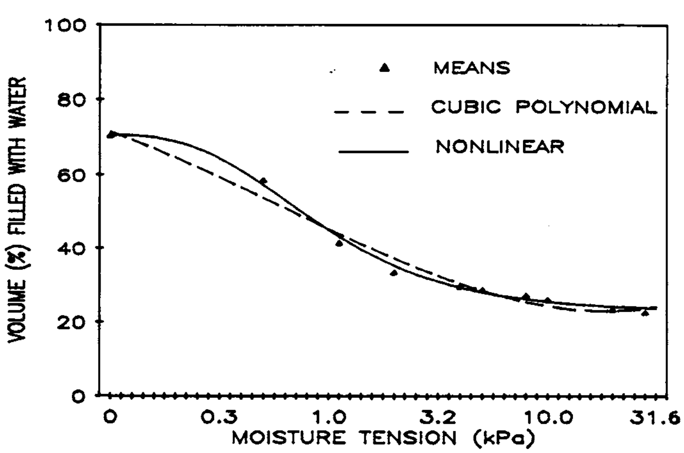

Fig. 3. Means and predicted moisture retention curves for cubic polynomial (Model I) and nonlinear (Model II) regression for medium 3 (3 bark : 1 peat : 1 sand).

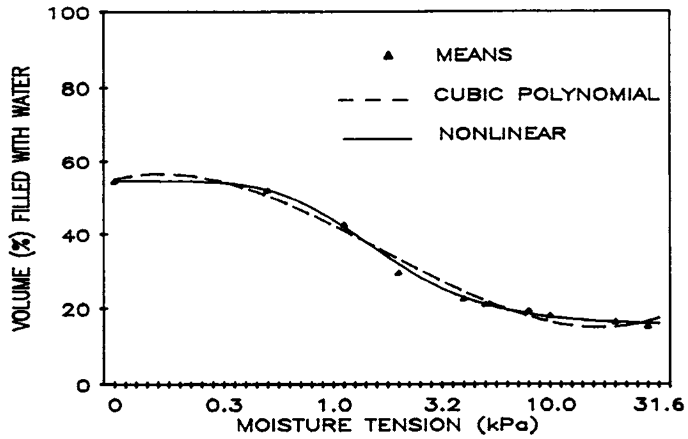

Fig. 4 Means and predicted moisture retention curves for cubic polynomial (Model I) and nonlinear (Model II) regression for medium 4 (1 soil : 1 peat : 1 sand).

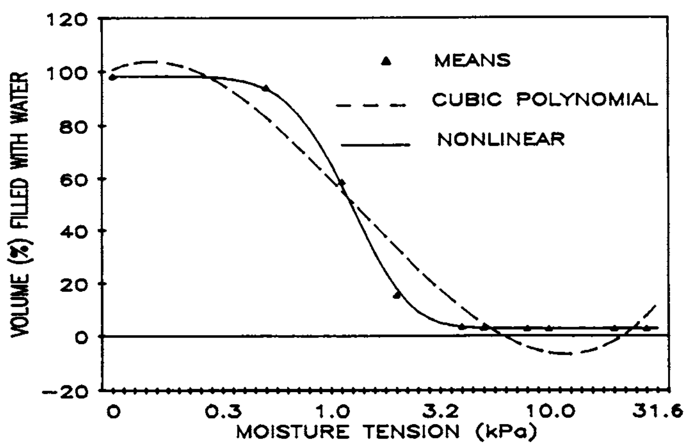

Fig. 5. Means and predicted moisture retention curves for cubic polynomial (Model I) and nonlinear (Model II) regression for medium 5 (phenolic foam).

mination for both the cubic (Table 2) and nonlinear models (Table 3). All SEs were small, except for the m values of the clay loam and foam (Table 3). We have found that large changes in this value often alter the model shape only slightly. The SE for Θ_s and Θ_r for the nonlinear model are 0, as these are known parameters and so did not have regression SEs. Mean square error (MSE) or mean square of residuals (an unbiased estimate of variance) was used to compare the models. For all media, except the clay loam, the nonlinear model had a lower MSE. The clay loam exhibited a characteristic curve with a shallow slope due to a polydisperse pore size distribution (Fig. 1) and was the most linear of the media tested. It was the only medium for which the cubic polynomial had a lower MSE. The coefficients of determination (r^2) (the model sum of squares divided by the total sum of squares) were high in all cases (>0.95), indicating that both models fit the data well.

The adequacy of each model to describe the experimental data was also evaluated using a lack of fit (LOF) test. An estimate of true error (error due to replication) was calculated by pooling the variances. Subtracting this value from the residual sums of squares yielded the LOF sum of squares. A significant F test (LOF mean square over the true error means square) indicates that a significant proportion of variance is due to an inappropriate or poorly designed model rather than the data itself. Calculated F (Table 4) values were much higher for the cubic polynomial for all media, except the clay loam, indicating that the nonlinear model was more appropriate. Only two LOF tests (both nonlinear models) were not significant. Most observations had very small true error due to the high precision of laboratory

Table 2. Parameter values, SEs (in parentheses), mean square errors (MSE), and coefficients of determination (r^2) for the cubic polynomial[z] (Model I) for five substrates.

Medium	Model parameters a	b	c	d	MSE	r^2
Cecil clay loam	60.7 (0.5)	−14.2 (1.8)	−6.5 (1.7)	2.6 (0.5)	1.9	.986
1 peat : 1 vermiculite	87.8 (1.0)	−11.5 (3.6)	−22.4 (3.5)	7.4 (0.9)	6.6	.981
3 bark : 1 peat : 1 sand	71.3 (0.8)	19.6 (2.8)	−10.9 (2.7)	4.5 (0.7)	5.3	.978
1 soil : 1 peat : 1 sand	55.0 (0.8)	14.6 (2.8)	−37.3 (2.7)	10.2 (0.7)	5.4	.975
Phenolic foam	100.8 (3.1)	35.0 (10.6)	−108.6 (10.3)	32.2 (2.7)	66.3	.956

[z] $Y = a + b + cX^2 + dX^3$

Table 3. Parameter values, SEs (in parentheses), mean square errors (MSE), and coefficients of determination (r^2) for the nonlinear function[z] (Model II) for five substrates.

Medium	Model parameters Θ_s	Θ_r	α	n	m	MSE	r^2
Cecil clay loam	61.5	25.0	0.3 (0.3)	1.8 (0.4)	8.2 (87.4)	2.3	.998
1 peat : 1 vermiculite	86.9	31.9	0.9 (0.1)	3.3 (0.2)	1.2 (0.8)	1.3	.999
3 bark : 1 peat : 1 sand	70.5	22.7	3.4 (0.6)	1.1 (0.1)	1.0 (0.6)	1.3	.999
1 soil : 1 peat : 1 sand	54.6	15.4	5.2 (0.6)	0.8 (0.1)	1.0 (0.3)	3.0	.997
Phenolic foam	98.3	3.0	6.3 (1.0)	0.7 (0.2)	4.7 (24.5)	1.9	.999

[z] $Y = (\Theta_s - \Theta_r)/[1 + (\alpha X)^n]^m + \Theta_r$.

Table 4. Lack of fit tests and residuals of predicted moisture retention curves using cubic polynomial and nonlinear regression for five media.

Regression equations	Lack of fit test: F statistic	Significance at the 0.05 level	Residuals[z]: High	Low	Mean (absolute)
		Cecil clay loam			
Cubic[y]	3.3	*	3.3	−2.7	1.1
Nonlinear[x]	5.2	*	2.3	−2.9	1.1
		1 peat: 1 vermiculite			
Cubic	90.1	*	6.1	−4.2	2.2
Nonlinear	9.6	*	2.1	−2.5	0.9
		3 bark : 1 peat : 1 sand			
Cubic	84.9	*	5.5	−4.7	1.8
Nonlinear	10.2	*	2.0	−2.8	0.9
		1 soil : 1 peat : 1 sand			
Cubic	11.5	*	4.6	−6.3	1.8
Nonlinear	1.1	NS	6.1	−4.2	1.3
		Phenolic foam			
Cubic	407.7	*	12.2	−19.5	6.6
Nonlinear	1.7	NS	5.2	−4.4	0.8

[z] Observed minus predicted as percent moisture (by volume).
[y] $Y = a + bX + cX^2 + dX^3$.
[x] $Y = (\Theta_s - \Theta_r)/[1 + (\alpha X)^n]^m + \Theta_r$.

procedures, hence the significant LOF. Observations of field data with the same means, but with larger true error, more often show nonsignificant LOF.

The assumption made for use of these models was that there was a normal distribution of independent random variables with common variances. To meet the assumption, all residuals must lie within ±2 SD. Residuals (observed minus predicted value) were calculated (Table 4) to check this assumption. The mean absolute values of the residuals were small for both models, except for the polynomial for the phenolic foam. Values for the nonlinear model were never larger than for the polynomial. The nonlinear model always had mean absolute residuals <2 (percent moisture). However, several residuals from both models exceeded the limit of ±2 SD (Table 4). There are two reasons for this. First, the data variances are heterogeneous (greater at low MT values), which is a function of the method used to collect the data. Second, residuals were correlated to observations. The polynomial showed a sigmoid pattern of residuals, while the nonlinear pattern relates to Θ_s and Θ_r. The curve was forced through the mean of Θ_s (therefore no variance) and used the investigators' choice of data for Θ_r (a point on the second plateau). If the slope at Θ_r is not 0, predicted values near Θ_r will be greater than observed values. For this reason, great care should be taken regarding the final pressure setting for each medium being tested. It should be noted, however, that greater model accuracy was achieved using a measured value for Θ_r, as suggested by Stephens and Rehfeldt (14), than by calculating Θ_r from the model, as described by Van Genuchten and Nielsen (18).

Validity of the models is illustrated in Table 5, where means of saturation and four ranges of the media's retention curves are compared to the corresponding values calculated using the two models. Values at saturation (0 kPa) for the nonlinear model are identical to the mean, by definition. The cubic model was accurate for all media except for the phenolic foam, for which it predicted saturation >100% (a physical impossibility).

The range 0 to 0.4 kPa corresponds to the water released upon drainage under atmospheric pressure (0.4 kPa is the average MT of the core at drainage). For all media, water contents predicted by the nonlinear model were closer to the observed water contents. The cubic model exhibited a 4-fold error for foam and predicted considerably inflated drainage values for peat-, bark-, and soil-based mixtures. In the range of 0.4 to 5 kPa, the nonlinear model still provided the best predictive curve.

The fourth column in Table 5 presents data in the range of 5 to 30 kPa. Data were collected to 30 kPa, with the aim of having a point on the second plateau of the curve. In spite of this, only the polymer foam data were sufficiently asymptotic at high MT that the nonlinear model did not over-estimate Θ in this range.

Table 5. Means and predicted values of percent by volume of water released at 0 kPa[z] soil moisture tension, and percent by volume held between 0 and 0.4, 0.4 and 50, 5 and 30, and 0.4 and 30 kPa soil moisture tension using cubic polynomial and nonlinear regression for five substrates.

Regression equations	Water content (% by volume) kPa 0	0–0.4	0.4–5	5–30	0.4–30
	Cecil clay loam				
Mean	60.5	10.3	19.9	6.2	26.1
Cubic[y]	60.7	11.9	18.6	5.7	24.2
Nonlinear[x]	60.5	9.5	21.0	4.9	25.9
	1 peat : 1 vermiculite				
Mean	86.9	10.7	36.2	8.0	44.2
Cubic	87.8	15.9	32.4	5.7	33.9
Nonlinear	86.9	11.3	36.8	5.1	41.9
	3 bark : 1 peat : 1 sand				
Mean	70.5	11.8	29.9	6.1	35.9
Cubic	71.3	17.0	25.9	4.4	30.3
Nonlinear	70.5	12.1	30.4	3.7	34.0
	1 soil : 1 peat : 1 sand				
Mean	54.6	2.6	30.9	5.8	36.7
Cubic	55.0	4.2	29.0	4.8	33.8
Nonlinear	54.6	2.0	31.6	4.6	36.1
	Phenolic foam				
Mean	98.3	4.1	90.2	0.2	91.2
Cubic	100.8	16.4	80.3	−6.2	74.1
Nonlinear	98.3	3.8	91.3	0.2	91.4

[z]1 kPa = 10.2 cm of H_2O = 0.01 bars.

[y]$Y = a + bX + cX^2 + dX^3$.

[x]$Y = (\Theta_s - \Theta_r)/[1 + (\alpha X)^n]^m + \Theta_r$.

Because of this, the cubic model provided the best estimates of means for all media within this region, except for the foam. If this portion of the curve is of particular importance, water content at a higher tension should be determined to give a better estimate of Θ_r.

The cubic model appears to fail for substrates, such as peat-based mixes and foam, whose curves have extended plateaus connected by a steep slope. It is apparent that the model used to describe characteristic curves needs to be adaptable to all types of media that are developed. The nonlinear model was both more versatile and more accurate than the cubic polynomial power series in describing water characteristics of various horticultural substrates.

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