Simulation Modeling of Temperatures in Root Container Media

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Abstract. A three-dimensional computer model was developed to simulate numerically the thermal environment of a polyethylene container-root medium system. An energy balance was calculated at the exterior container wall and the root medium top surface. Thermal energy exchanges at the system’s boundaries were a function of radiation, convection, evaporation, and conduction energy fluxes. A forward finite difference form of a transient heat conduction equation was used to calculate rates of temperature changes as a result of thermal energy exchanges at the system’s boundaries. The χ2 “goodness-of-fit” test was used to validate computer-generated values to actual measured temperature data. Probabilities for the null hypothesis of no association ranged from $P = 0.45$ (Julian day 271), to $P = 0.81$ (Julian day 190), with $P ≥ 0.70$ on nine of 10 validation days in 1989. Relative to net radiation and convection, evaporation and conduction had little effect on thermal energy exchanges at the root medium top surface during sunlight hours. The rate of movement of thermal energy (thermal diffusivity) was slower and generally resulted in lower temperatures in a pine bark medium than in a pine bark medium supplemented with sand when volumetric water content (VMC) ranged from 0.25 to 0.45.

Researchers have attempted to characterize temperature patterns in container media (Fretz, 1971; Martin and Ingram, 1988a; Pertuit, 1972; Young and Hammett, 1980). However, the relationship of environmental factors and medium physical properties to temperature patterns in container media profiles has proven difficult to establish from field experimentation. Development of analytical solutions to predict temperatures in container media systems as a function of these relationships is difficult to traditional field studies, simulation models expand the researcher’s capacity to study responses of all relevant factors. Information gleaned from simulations can depict the dynamic nature of microcosms inside a container medium profile. Thus, a simulation model would help to identify cultural management practices that reduce medium temperatures below critical levels for root survival.

The primary environmental factors causing changes in container medium temperature patterns are solar radiation, wind, air temperature, and absolute air humidity. Root medium temperatures as high as 57°C have been recorded adjacent to container walls exposed to solar radiation (Martin and Ingram, 1988a). Rooting patterns of Magnolia grandiflora Hort. ‘St. Mary’, grown in black polyethylene containers exposed to solar radiation, varied with season and exposure duration (Martin et al., 1991). Convection energy flows are caused by wind interacting with the temperature differential between the container system’s boundary and surrounding air (Churchill and Bernstein, 1977). Moisture gradients between the top surface of the medium and surrounding air cause thermal energy flows due to the latent heat of vaporization or condensation (Enz et al., 1988).

Medium composition influences thermal diffusivity because of the differing thermal properties, e.g., thermal conductivity, bulk density, and specific heat capacity of the individual components (Parikh et al., 1979; Sophocleous, 1979). A root medium’s water content can also affect thermal diffusivity (Martin and Ingram, 1991). Our objectives were to develop and validate a three-dimensional computer model to simulate container root medium temperature patterns. We used the model to investigate the relative influence of net radiation, convection, evaporation, and conduction on thermal energy exchanges at the top surfaces of the medium and research the effect of volumetric moisture content (VMC) on medium temperature patterns for three growth media in 10-liter containers.

Materials and Methods

System description and model development. The model system consisted of two components: 1) a cylindrically shaped, polyethylene container (0.0235-m top diameter, 0.023-m bottom diameter, 0.023-m height, and 0.0025-m wall thickness) filled with 2) a soilless root growth medium containing combinations of milled pine bark, sieved through a 0.0125-m screen, and builder’s sand [pine bark only, 4 pine bark : 1 sand (v/v); and 3 pine bark : 2 sand (v/v)]. Milled pine bark and builder’s sand were chosen because they are frequent components of outdoor container production media and because they have thermal properties representative of some organic and mineral inorganic materials, respectively, comprising soilless mixes for outdoor container production.
temperature changes at any point in the system were calculated using partial differential equations (Holman, 1986; Hornbeck, 1975). Thermal energy flows across the container wall were assumed to occur one-dimensionally. This assumption was made with consideration given to the thermal properties of polyethylene (Baer, 1975) and the container dimensions. The rate of temperature change across the container wall was defined as

\[ \frac{\delta T}{\delta t} = \text{ALPHA}(\delta^2 T/\delta x^2) \]  

where \( T \) was temperature (C), \( t \) was time (seconds), \( \text{ALPHA} \) was thermal diffusivity (m²/s), and \( x \) was container wall thickness (m). Therefore, wall temperatures depended on polyethylene \( \text{ALPHA} \), wall thickness, and temperature differentials between the outer and inner wall surfaces in the horizontal dimension. Thermal energy flows within the medium were assumed to occur three-dimensionally and were defined as

\[ \frac{\delta T}{\delta t} = \text{ALPHA}(\delta^2 T/\delta r^2 + 1/r(\delta T/\delta r)) + \delta^2 T/\delta z^2 \]  

where \( r, \beta, \) and \( z \) were the radial, angular, and vertical coordinates, respectively, of the point of temperature calculation. Medium \( \text{ALPHA} \) was based on empirically determined (Martin and Ingram, 1991) or previously derived values of thermal conductivity (K), bulk density (RHO), and specific heat capacity (CP) of the constituent parts. Medium K was measured with a TC-1 conductivity probe (Decagon Devices, Inc.; Pullman, Wash.) connected to a 21X micrologger (Campbell Scientific, Logan, Utah). Medium RHO was measured as the average weight per volume of the pine bark, sand, and water comprising each medium. Thermal properties of polyethylene were obtained directly from handbooks (Baer, 1975), whereas CP values for pine bark, sand, and water were obtained from tables of thermal properties and weighted according to the percentage volume of each component (Raznjievic, 1976; ASHRAE, 1989). \( \text{ALPHA} \) was then calculated as

\[ \text{ALPHA} = K/[(\text{RHO})\text{CP}] \]  

Predictive, equations for K and RHO were developed previously to model \( \text{ALPHA} \) as a function of volumetric water content (Martin and Ingram, 1991). Our simulation model can predict the thermal response of other material and root media equally well if only their thermal properties are known.

A forward finite difference form of Eqs. [1] and [2] was used to predict the rates of temperature change during computer simulation (Holman, 1986; Hornbeck, 1975). To expedite finite difference extrapolation, the model system was partitioned into discrete subunits. The medium was segmented in the vertical dimension into 10 separate layers. Each layer contained 97 discrete subunits of thermal energy storage of 0.0135-m diameter and 0.02-m height. The polyethylene container was segmented into 289 subunits: 192 in the container wall (0.0025-m diameter, 0.02 m high) and 97 in the container bottom (0.0135-m diameter, 0.0025 m high). Therefore, the model system consisted of 1257 energy storage subunits, each having a single uniform temperature at any time (t). Euler integration was used to predict temperatures at all internal system subunits (Hornbeck, 1975).

Net radiation energy (NRAD) flows were divided into three components (Robinson, 1966): 1) direct beam solar radiation (IDN), 2) diffuse radiation (ID), and 3) longwave radiation (IL). Values for IDN were either received directly from historic meteorological data or were model-generated based on an assumed sinusoidal pattern of IDN to time of day as

\[ \text{IDN} = \text{IDNMAX}[\sin(TD/TC)] \]  

where \( \text{IDNMAX} \) was maximum potential direct beam radiation (W·m⁻²) at solar noon based on latitude, Julian day, and an assumed atmospheric turbulence coefficient of 0.85 (Flint and Childs, 1987). \( TD \) was the time (seconds) expired since sunrise, and \( TC \) was the total potential duration (seconds) of sunshine. Values of ID and IL were calculated using equations from van Bavel and Hillel (1976). Values for NRAD were then calculated as

\[ \text{NRAD} = [(1 - \text{ALB})\text{IDN}] + \text{ID} - \text{IL} \]  

where \( \text{ALB} \) was surface albedo or reflective capacity. Different values for \( \text{ALB} \) were used for the container wall and medium top surface; for the wall, \( \text{ALB} \) depended on container color and was held constant during a simulation run. For the medium top surface, \( \text{ALB} \) varied as a function of the VMC (Chung and Horton, 1987; Linacre, 1969) and was calculated as

\[ \begin{align*}
\text{ALB} &= 0.25, & & \text{for } \text{VMC} \leq 0.10 \\
\text{ALB} &= 0.35 - \text{VWC}, & & \text{for } 0.10 \leq \text{VMC} \leq 0.25 \\
\text{ALB} &= 0.10, & & \text{for } 0.25 \leq \text{VMC}.
\end{align*} \]  

For convection energy flows, if wind speed was \( \geq 1.0 \) m·s⁻¹, then heat transfer coefficient (H) values were calculated via correlations of experimental data for turbulent gaseous crossflow according to Hilpert (1933). If wind speed was \( \leq 1.0 \) m·s⁻¹, then H values were calculated for the polyethylene container and container medium surface based on equations for natural convection according to Gebhart (1970) or Churchill and Chu (1975), respectively. Thermal energy flows from and to external boundaries due to convection were a function of temperature differentials (\( \delta T \)) between ambient air and convecting surfaces multiplied by the appropriate convection heat transfer coefficient, or \( H(\delta T) \). For the latent heat of evaporation or condensation, diffusive water movement in the container medium profile was assumed to occur in the vapor phase only. Thus, mass transfer of water in the model occurred from the evaporation front to the surrounding atmosphere as a function of the absolute humidity and temperature differentials between the evaporating surface and the surrounding air and the atmospheric turbulence coefficient of resistance (Enz et al., 1988; Lamoreux, 1962; Thorn and Oliver, 1977; van Bavel and Hillel, 1976).

The model system included one internal and two external boundaries. The rate of temperature change at the internal boundary (i.e., the polyethylene container–root medium interface) was assumed to occur instantaneously. At external boundaries, temperature was defined explicitly at each time (t) via calculation of an energy balance. Thermal energy was exchanged between the system and surrounding environment by NRAD, convection, and evaporation at the medium top surface and by NRAD and convection at the exterior wall. Thermal energy moved throughout the medium volume via conduction. Accordingly, the external boundary equation for the medium top surface was

\[ Y_m = [\text{NRAD} - \text{EH} + (H_m)(T_m) + ((K_m)Y_{2m})/dM] + H_m + K_m / dM \]  

where \( Y_m \) and \( Y_{2m} \) were growth medium temperatures at the medium top surface and 0.01 m below the medium top surface, respectively, EH was the latent heat of evaporation or condensation (W·m⁻²·K⁻¹), \( H_m \) was the heat transfer coefficient (W/m²·K) for the top surface of the medium, \( T_m \) was air tem-
perature (C), \(K_w\) was medium thermal conductivity (W/m·°C), and \(d M\) was the distance (m) between \(Y_i\) and \(Y_n\). The external boundary equation for the exterior wall was

\[
\text{CONOUT}_{jn} = \left[ \text{NRADP} + \left( \frac{H_u (T_u)}{2 (K_p + K_w) / dP} \right) \right] / \left( H_p + K_p / dP \right) \tag{8}
\]

where \(\text{CONOUT}_{jn}\), and \(\text{CONIN}_{jn}\), were the temperature (C) of the outer and inner container wall, \(\text{NRADP}\) was net radiation (W/m²) incident on the polyethylene wall oriented perpendicular to the ground, \(H_u\) was the heat transfer coefficient of polyethylene (W/m²·°C), \(K_w\) was thermal conductivity of polyethylene (W/m·°C), and \(d P\) was container wall thickness (m).

**Simulation and validation.** Input data for simulation included local latitude and longitude, local standard time meridian, and Julian day. During simulations, new values of \(T_a\), wind speed, relative humidity, and IDN were used in the model during each 15-min continuous simulation interval. Computer algorithms were constructed to provide options for 1) use of historic meteorological data, 2) holding any combination of input values constant, or 3) allowing the model to calculate meteorological data via an assumed physical relationship. For historic meteorological data, a standard meteorological observation unit (Wallace and Hobbs, 1977) was constructed to monitor environmental factors. Solar radiation was recorded by a LI-COR 200SZ pyranometer sensor (LI-COR, Lincoln, Neb.). Relative humidity and \(T_a\) were recorded by a Model 207 sensor (Campbell Scientific). Wind speed and direction were recorded by a Model 014A anemometer and Model 024A sensor, respectively (Campbell Scientific). Computer-generated \(T_a\) values required daily maximum and minimum temperatures that were obtained from the WGEN model for generating daily weather variables (Richardson and Wright, 1984). Diurnal fluctuations of \(T_a\) were assumed to follow a sinusoidal pattern and were calculated as

\[
T_s = \left[ \frac{1}{400} \left( T_{\text{max}} - T_{\text{min}} \right) \right] + T_{\text{min}} \tag{9}
\]

where \(T_{\text{max}}\) and \(T_{\text{min}}\) were the daily maximum and minimum air temperatures (C), respectively.

The pivotal steps for simulation of root medium temperatures in a container are shown as a flow diagram (Fig. 1). During each 15-min continuous simulation interval, calculations were also made for \(H_u\) and medium VMC as a function of the evaporative water loss from the medium surface. These values were used to solve for external boundary temperatures with Eqs. [7] and [8]. Next, Eq. [1] was solved to predict the polyethylene container temperature profile. Then, Eq. [2] was solved for each energy storage subunit to predict the medium temperature profile.

Validation data were recorded for 24 h (0 to 2400 hr) on 10 meteorologically unique days during 1989 (Julian days 172, 173, 190, 191, 242, 243, 270, 271, 340, and 341) in Gainesville, Fla. (latitude 29.4°N, longitude 82.2°W). The weather conditions were selected to be highly variable among dates to provide a rigorous test of the predictive capabilities of the computer model. Gainesville has a subtropical climate characterized by mild, dry winters and hot, wet summers. Black polyethylene 10-liter containers were filled with milled pine bark previously sieved through a 0.0125-m screen and placed, 0.12 m apart, on a black polypropylene ground cover. Root medium temperatures were recorded using copper-constantan thermocouples connected to a 21X micrologger with AM-32 multiplexer (Campbell Scientific). Thermocouples were positioned in the medium 0.11 m below the medium top surface at the center location and on the north, east, south, and west coordinates, 0.02 m inside the container wall. Thermocouples were also positioned at the medium bottom and surface, 0.02 m above the container bottom and 0.02 m below the medium surface. Thermocouple positions were replicated in five containers on each validation date. Each pot was irrigated to container capacity the day before (1800 to 2000 hr) temperatures were recorded. The \(\chi^2\) method was used to test "goodness-of-fit" (Steel and Torrie, 1980) of computer-generated to actual measured medium temperatures across thermocouple positions for a 24-h simulation (Neelamkavil, 1987). Pearson's correlation coefficients were used to correlate computer-predicted with mean recorded medium temperatures for the previously defined thermocouple positions from simulation data from 0600 to 2100 hr on each validation date (Snedecor and Cochran, 1980).

**Model applications.** The effect of environmental factors and system characteristics on medium temperature patterns were studied by changing factors or characteristics alone or in factorial combinations during simulation runs. Thermal energy flows were modeled in 10-liter containers because conventional nursery production practices, for this size container and larger, often require container spacing at distances that subject their walls to direct solar radiation. The relative capacity of net radiation, convection, evaporation, and conduction to regulate thermal energy flows were investigated by simulating an energy balance at the medium top surface. Simulations of the energy balance were generated using historic meteorological data for Gainesville for Julian days 201 (partly cloudy evening, hot) and 341 (mostly cloudy, mild) in 1989.

The effects of VMC and medium composition on temperature patterns within the medium profile were studied with simulations that modeled VMC as a continuous parameter (0.1 to 0.7 at 0.05 intervals) for the three growth media. The simulations were generated for Julian day 206 (assumed clear, hot) using model-generated meteorological data for direct solar radiation and constant wind speed (2 m·s⁻¹) and 50% constant relative humidity.

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*Fig. 1. Simplified flow diagram of the computer model. Computer programs were written in Turbo Pascal 5.5-for microcomputer applications. Simulations were on a CompuAdd 386-25 personal computer (CompuAdd Co., Austin, Texas) with an 80386 math coprocessor.*
Results and Discussion

Validation. There was no statistical difference between computer-generated and actual measured temperatures (Table 1). Chi-square probabilities for the null hypothesis of no association between computer-predicted and mean recorded root medium temperatures across five locations for each validation date ranged from $P = 0.45$ (Julian day 271) to $P = 0.81$ (Julian day 190), with $P \geq 0.70$ on nine of the 10 validation days.

We selected three meteorologically disparate dates (Julian days 191, 243, and 341) to study the correlation of computer-generated and actual measured temperature data at the five medium locations. For Julian day 191 (8 July 1989), the weather was mostly sunny and hot with a $T_{\text{max}}$ of 36.3°C at 1400 HR. For this date, the center location will be discussed because the mean recorded temperature was maintained > 40°C from $1415$ to 2015 HR. For Julian day 243 (31 Aug. 1989), the weather was mostly sunny during the morning and early afternoon and partly to mostly cloudy during the late afternoon with a $T_{\text{max}}$ of 35.4°C at 1345 HR. The east and west coordinates will be discussed because the mean recorded $T_{\text{max}}$ were high and large differences in morning and afternoon radiation fluxes demonstrated the model’s correct calculation in response to abrupt changes in environmental input data. For Julian day 341 (7 Dec. 1989), the weather was partly to mostly cloudy all day with a $T_{\text{max}}$ of 23.7°C at 1530 HR. The north and south coordinates will be discussed because during late fall and winter, the solar declination angle is low and the highest medium temperatures typically occur on the southern exposure adjacent to the container wall (Martin and Ingram, 1988a).

For Julian day 191, predicted medium temperatures at the center location were consistently within 1 SE of the mean recorded temperature (Fig. 2). Mean recorded temperature SES were greater during late morning to midday than at other times during the day. This tendency occurred on most validation dates for the center location and was probably due to slight deviations in the thermocouple placement in the medium. For other validation dates, computer-predicted temperature patterns at the center location were also generally highly correlated to mean recorded temperatures; however, predicted and recorded temperatures were more highly correlated during summer than in fall or winter. Pearson’s correlation coefficients at the center location for all validation dates ranged from $r = 0.86$ on Julian day 271, to $r = 0.99$ on Julian day 191.

For Julian day 243, computer-predicted medium temperatures at the east coordinate were generally 1 to 2°C higher than mean recorded (OBS) temperatures from 1600 through 2100 HR, but were within 1 SE of mean recorded values earlier in the simulation (Fig. 3A). Variations in the SES of mean recorded temperatures followed trends similar to the center location (Fig. 2) and were also probably due to variation in thermocouple placement. Increased SES were most common during periods of rapid temperature fluctuations resulting from exposure of the east-facing container walls to solar radiation. For other validation dates, predicted container medium temperatures at the eastern coordinate were generally highly correlated with mean recorded temperatures. Pearson’s correlation coefficients for validation dates ranged from $r = 0.82$ on day 191 to $r = 0.99$ on Julian day 340.

Correlations of temperature patterns at the west coordinate (Fig. 3B) were similar to those for the center location (Fig. 2). For day 243, computer-predicted temperatures were generally within 1 SE of mean recorded values (Fig. 3B). Predicted temperatures were more highly correlated with mean recorded temperatures during summer than in fall or winter. Pearson’s correlation coefficients at the western coordinate for all validation dates ranged from $r = 0.86$ on Julian day 271 to $r = 0.99$ on Julian day 172. Lower correlations during fall and winter were due consistently to the model’s underestimated of daily maximum temperatures.

For Julian day 341, computer-predicted medium temperatures for the north and south coordinates were =0.5 to 2°C higher than mean recorded temperatures from 1800-2100 HR (Fig. 4). For other validation dates, predicted temperatures at the northern and southern coordinates were highly correlated with mean recorded temperatures. Pearson’s correlation coefficients at the north and south coordinates for each validation date ranged from $r = 0.95$ on Julian day 270 to $r = 0.99$ on Julian day 173 and from $r = 0.92$ on Julian day 242 to $r = 0.99$ on Julian day 173, respectively. In general, the correlation coefficients at the north coordinate were higher than at the east, south, and west coordinates, and were higher than those at the center location. This result is not surprising since daily temperature fluctuations at the north exposure of a nursery container are usually smaller than other exposures, as the north container wall is least exposed to direct solar radiation.

Overall, the model predicted medium temperatures best when simulations were conducted with summertime environmental variables. Computer-generated temperatures were usually within 1 SE of actual measured temperatures. Overestimation of temperatures was more common during late fall and winter, as the north container wall was least exposed to direct solar radiation.
Fig. 3. Mean recorded (OBS) and computer-predicted (PRE) container root medium temperatures in a 10-liter container filled with milled pine bark at the (A) east and (B) west coordinates for Julian day 243 (31 Aug. 1989). Copper-constantan thermocouples were positioned halfway down the medium profile, 2 cm inside the container wall. Bars attached to OBS are ±1 se, n = 5.

Temperatures at the south coordinate after the daily maximum temperature had occurred and underestimation of the maximum daily temperature at the western coordinate during fall and winter months were the principal sources of variation between behavior of the model and real systems. Model characteristics were calibrated to real system temperature patterns for summer, which might account for differences between computer-generated and actual measured temperatures during the fall and winter. However, validation tests revealed that behavior of the model system was always statistically and qualitatively similar to the real system, consequently, the computer model could be used for evaluation of factors that influence the incidence of high temperature-induced root injury of container-grown plants.

Model application. Simulations of an energy balance at the root medium top surface for Julian days 201 and 341 indicated that the principal physical processes that affected temperature patterns at the medium surface were net radiation and convection (Fig. 5). During sunlight hours, conduction and evaporation had little effect on thermal energy flows to and from the medium top surface. Energy balance calculations show that the primary energy source to the medium surface was insolation and the primary energy sink from the medium surface was the surrounding atmosphere. For Julian day 201, fluctuations in net radiation and convection values between 1200 and 1400 HR were caused by increased cloud cover. Lower negative convectional energy values at 1915 HR were caused by increased wind speed (0.44 to 3.68 m·s⁻¹) (Fig. 5).

Changes in medium temperature patterns adjacent to the container wall, induced by medium composition or VMC, were negligible (<1°C). However, there appeared to be an interaction of medium composition and VMC with changes in temperature at the medium’s center location (Fig. 6). As VMC ranged from 0.1
to 0.7, the degree hours > 40°C for the 3 pine bark : 2 sand (Fig. 6C) and 4 pine bark : 1 sand (Fig. 6B) media increased linearly from 9.8 to 15.4 C/h and from 10.6 to 12.4 C/h, respectively. For these two root media, increased VMC also increased the duration > 40°C from 5.25 to 6.75 h and from 5.5 to 5.75 h, respectively, and the daily amplitude from 42.9°C (2030 HR) to 44.0°C (1945 HR) and from 43.2°C (2030 HR) to 43.4°C (2015 HR), respectively. These differences could be mostly attributed to changes in medium values for K as VMC was increased.

Temperature patterns at the center of pine bark (Fig. 6A), as a function of VMC, were different when contrasted with the pine bark media supplemented with sand (Fig. 6B, C). Although the daily amplitude was 42.2°C (2100 HR) when VMC = 0.1, the daily amplitude failed to exceed 40°C when VMC = 0.25. This difference between media is significant since Ingram et al. (1989) reported the need for nursery operators to be cognizant of root zones > 40°C. Also, 90% and 50% of unacclimated Magnolia grandiflora ‘St. Mary’ and Ulmus parvifolia Hort. ‘Drake’ test plants, respectively, were killed during 12 weeks of exposure of the root zone to 42°C for 6 h daily (Martin and Ingram, 1988b). However, if VMC ranged from 0.55 to 0.70, then temperature patterns at the center of the pine bark were similar to those for the pine bark supplemented with sand. These differences could be attributed mostly to changes in growth medium RHO and CP as VMC was increased from 0.1 to 0.45, and changes in K as VMC was increased from 0.45 to 0.7 (Martin and Ingram, 1991; Raznjevic, 1976).

Overall, container medium ALPHA increased as VMC increased. This resulted in root media that warmed faster and earlier in the day but also cooled faster at night. During periods of hot, dry weather, 10-liter containers in outdoor production nurseries are often watered daily. For a pine bark medium, nursery operators might maintain VMC ≤ 0.45 from 1000 to 1800 HR to moderate the influx of thermal energy into the container medium profile. Under these conditions, irrigations might be applied in the afternoon. This strategy would allow irrigations to function as a tool for direct thermal energy dispersal, as well as permit maximum time for VMC to decrease before the irrigation the following day. This management strategy, however, would appear to be less important for pine bark medium supplemented with sand.

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