Framework for mathematical modeling of Soil-Tree system

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Abstract A systemic framework for mathematical modeling of Soil-Tree system is proposed through this work. The model couples the vadose zone moisture uptake by trees with the cumulative multi-layered canopy water demand. The water demand is estimated by integrating the photosynthesis models and stomatal conductance with the leaf energy balance. The philosophy of the modeling framework is to portray the tree as a living entity which continuously interacts with the dynamic micro-climatic variables only to economize the biomass production at the cost of transpiration. The model can quantify the changes in transpiration patterns due to various climate change scenarios and comes in handy to perform ‘*what-if?*’ kind of theoretical experiments on trees.

Keywords Soil-Plant system · Stomatal conductance · Mathematical modeling · Vadose zone · Water demand · Micro-climatic variables

Introduction

With a change in climatic variables there can be an altered behavior of vegetation in terms of its CO₂ intake and H₂O uptake. Researchers are curious to study the behavioral patterns of vegetation due to the climate change. Capra (1996) has stated that, according to Gaia theory and Daisy-world models, both abiotic and biotic components of earth

would equilibrate imbalances prevailing between them; leading towards a new order of world. In a holistic view, it can be said that, with the change in climate, there can be an altered behavior of vegetation, and similarly the change in vegetation behavior would also affect the climate. For instance, according to Katul et al (2010), the decrease in stomatal conductance of trees would result in decrease in its transpiration rates—which eventually accelerates surface water runoff.

Nevertheless, an attempt can be made to study a part of the changed responses of vegetation with the help of mathematical models—based on systems approach. Models made of *mechanistic approach* with a flavor of *systems theory* are highly appreciated as a research tools for testing the hypotheses on tree behavior in various climate change scenarios. The purpose is justified only when these models are able to capture the instantaneous behavior of trees with respect to the dynamic weather and soil conditions.

In 1970s and 1980s the mathematical models developed were either to mimic photosynthesis processes (Jarvis 1976; Farquhar et al 1980; Caemmerer and Farquhar 1981) or root water uptake (Belmans et al 1983; Landsberg and McMurtrie 1984; Feddes et al 1988; Steudle and Peterson 1988) or micro-climatic interactions with canopy (Knipling 1970; Collares-Pereira and Rable 1979; Howell and Meek 1983; Frouin et al 1989) etc., and those works remained in isolation. Earlier models were specific to a particular phenomenon, rather their objective was not to provide a complete picture of tree interactions with the environment. Shawcroft et al (1974) has also mentioned in agreement that, the common practice in earlier modeling was to model separate components of energy exchange systems. Nevertheless, these isolated works have paved the path for the *holistic models* which are developed subsequently.

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Later with the advent of *systems theory* ideology and enhanced computational facilities, ecologists were interested to model the whole forest level processes by connecting tree physiology with bio-geo-chemical nutrient cycles. The idea to mimic whole forest level processes was not that simple, because of multitude of environmental components and dynamic feedback mechanisms among them. Above all, the ecosystem is thermodynamically open and non-linear in nature (Wu and Marceau 2002). Some of the forest level process-based ecosystem models include the works of Aber et al (1995), Kimball et al (1997), Friend et al (1997), Wang et al (2001), Peng et al (2002) and Nikolov and Zeller (2003). Though, the forest level models have tried to capture the entire working pattern of an ecosystem, they lacked the subtlety of interactions. These trade-offs between quantity and quality are always inevitable with any of the ecological models.

However, there are other kinds of models which are specific to the physiology of a tree devoid of ecological dynamics of the forest. Most of these models are built on the philosophy of Soil-Plant-Atmosphere-Continuum (SPAC) to provide a complete tree level interactions/responses with the immediate environment (micro-climate/soil characteristics). Some of the SPAC models includes the works of Shawcroft et al (1974), Thorpe et al (1980), Landsberg and McMurtrie (1984), Tiktak and van Grinsven (1995), Williams et al (1996), Tuzet et al (2003) and Lee and Park (2007). Relative to ecological models, the scope of SPAC models is narrower, yet provides an insightful understanding regarding the behavior of a tree. Most of the SPAC models are *steady state* mathematical formulations with much of empiricism and treated the trees in compartments—one portion of the model leads to another in a sequential manner, which essentially misses the non-linearity of interactions and complex feedback mechanism. Although Tuzet et al (2003) could simulate the dynamic plant behavior it lacks the multi-layered differential treatment of canopy and they have used the semi-empirical models for stomatal conductance.

Through this model, a robust connection has been established between all other sub-models that have been dealing with trees and vadose zone in bits and pieces. The approach of the proposed model is novel in connecting the complex Soil-Tree system with non-steady state equations in a deterministic manner and by considering the multiple feed-back loops from micro-climatic and soil variables. The model is presented in a generic mode which helps as a research tool when scientists are interested to test the hypothesis based on *what-if* kind of experimentation on dynamic behavior of trees. Subsequently the model provides the means of a working engine for developing holistic ecological models.

Model description

Concept of the model

The model establishes the continuity in movement of water right from the pores of soil matrix till the tip of leaf and finally into the atmosphere. The atmosphere plays a role of sink, while the soil acts like a source of water letting the tree to economize how much water it has to uptake per unit of CO₂ intake. Nearly 98 % of the water uptake by the roots is lost in transpiration through the stomata. The stomata plays a dual role of allowing loss of water as well as absorption of CO₂. It is been emphasized by many researchers that, stomatal regulation is crux of the tree behavior. The ambiguity in quantifying the interplay of stomatal regulation is tackled in this model by connecting the feedback signals between leaf temperature, transpiration, leaf bio-chemical reactions and the stomatal conductance (concept diagram shown in Fig. 1).

As the micro-climatic driving variables constantly interact with the leaves present at different canopy layers, the respective demand for CO₂ intake and H₂O losses are generated. To quantify the photosynthesis and transpiration process along the depth of canopy, it is essential to establish the distribution of leaf area as a function of tree height (Landsberg and McMurtrie 1984). Similarly, the vertical distribution of meteorological driving variables along the depth of canopy is also equally important. These dynamic relations, with a multitude of driving and determining variables are inter-connected to arrive at the instantaneous water demand by the tree, which is to be drawn from the vadose zone (Fig. 2).

The sub-models describing various processes related to the tree (Fig. 1) viz. canopy structure, radiation regime, leaf boundary layer conductance, leaf biochemical reactions, stomatal optimization, flow of water and root water uptake etc. are elaborated in the following sections.

Canopy structure

Each layer of canopy receives different amount of solar radiation and wind speed. In order to capture the differential treatment, the canopy structure of the trees is divided into several horizontal layers with equal spacing from bottom height of canopy, H_b , to the top height of canopy, H_t . The amount of leaf area allocated in each layer is based on the tree skeleton (Chen et al 1994; Berezovskaya et al 1997) and Leaf Area Index (LAI).

LAI is the total one-sided area of leaf tissue per unit ground surface area (Breda 2003),

Fig. 1 Concept diagram for the proposed modeling framework **Fig. 2** Approach for the proposed model. Water demand is governed by the canopy level processes, that has to be balanced with root water uptake

$$LAI = \frac{\sum a_i}{A_c}$$

where a_i is area of individual leaf and A_c is vertical projection area of canopy on ground. LAI drives both the within and the below-canopy micro-climate, radiation extinction, H₂O and CO₂ gas exchanges. Therefore, LAI is a key component in bio-geo-chemical cycles in ecosystem (Ewert 2004). Teske and Thistle (2004) have applied the Weibull distribution functions to estimate the depth-wise distribution of LAI, which inherently takes care of fractal structure of tree canopy,

$$LAI_z = LAI \left(1 - \frac{1 - \exp \left[- \left[\frac{1 - (z/H_t)^c}{b} \right] \right]}{1 - \exp \left[- \left(\frac{1}{b} \right)^c \right]} \right) \quad (1)$$

where b and c are Weibull distribution parameters (depends on type of vegetation) and z is vertical axis positive along the length of tree.

Radiation regime

Radiation falling above the canopy

Hourly solar radiation falling on the top of the canopy with the assumption of clear sky condition, is derived from the work of Al-Rawahi et al (2011), which is acceptable when field measured solar radiation values are not available. Nevertheless, the radiation values measured at nearby meteorological stations would suffice. Total hourly solar radiation falling on the horizontal surface above the canopy, I_{th} , can be estimated from daily global radiation measurements, H (Duffie et al 1991),

$$I_{th} = \frac{r \times H}{3.6} \quad (2)$$

r is the ratio of $\frac{I_{th}}{H}$ as given by (Collares-Pereira and Rabl 1979),

$$r = \frac{\pi}{24} (a + b \times \cos(W)) \left[\frac{\cos(W) - \cos(W_s)}{\sin(W_s) - \frac{\pi}{180} W_s \cos(W_s)} \right]$$

where, W is hour angle of the sun, and W_s is sunset hour angle (dependent on latitude of the location), the expressions for a and b are provided in Appendix A.

Radiation attenuation due to canopy structure

The interception of incident solar radiation is dependent on the quantity of solar radiation, optical properties and density of the tree elements and canopy architecture (Chen et al 1994). Beer's Law is applied to determine the solar radiation absorbed in each canopy layer (Amthor 1994). The incident radiation flux declines exponentially with the depth of canopy, because of LAI_z (Niinemets 2010) i.e. encountered in the optical path of light. Canopy leaf angle arrangements

are not considered for the simplification of the model and reflection and refraction of incident solar radiation on canopy layers are neglected, instead attenuation is grossly considered through extinction factor. From the Eqs. (1) and (2), the amount of solar energy being received at a particular canopy layer, Θ_z , is approximated as

$$\Theta_z = I_{th} \times \exp(-k \times LAI_z) \quad (3)$$

where k is light extinction factor, which is obtained by comparing solar radiation intensities both above- and below-canopy.

Leaf boundary layer conductance

Leaf boundary layer is the still layer of air surrounding the leaf surface. The width of the layer depends on the wind-speed and leaf surface properties and shape. For transpiration to occur, the water-vapor leaving the stomata must diffuse through this motionless layer to reach the atmosphere. More the thickness of leaf boundary layer, higher the resistance the layer offers to the transpiration and as well as CO₂ uptake through the stomata. The ease with which boundary layer allows the transfer of mass is quantified in terms of conductance values. The quantification of boundary layer conductance as a function of wind-speed, U_z , and effective leaf length, l_e (usually diagonal leaf length), are adapted from Williams et al (1996).

Wind-speed, U_z , within the canopy layer, z , follows the exponential decay profile (Cionco 1985)

$$U_z = U_{top} \times e^{\left(\alpha \left(\frac{z}{H_t} - 1 \right) \right)} \quad (4)$$

where U_{top} is above-canopy wind speed and α is canopy flow index. Within each canopy layer the thickness of leaf boundary layer, δ , is derived using the relationship from the work of Nobel et al (1983);

$$\delta = 0.004 \sqrt{\frac{l_e}{U_z}} \quad (5)$$

where l_e is effective leaf length. Using Eq. (5), the g_h , boundary layer conductance to the heat transfer from the leaf surfaces can be related with thermal diffusivity in air, D_h , as

$$g_h = 2 \times \frac{D_h}{\delta}. \quad (6)$$

Leaf level processes

Gas diffusion

Mass transfer of CO₂ and H₂O between leaves and the atmosphere can be described by *Fickian diffusion* through the stomata [Eqs. (7), (8)]

$$f_c = g_s(C_a - C_i) \quad (7)$$

$$f_e = ag_s(e_i - e_a) \approx ag_s D \quad (8)$$

where f_c is CO_2 flux, f_e is the H_2O flux, g_s is stomatal conductance to CO_2 , C_a is ambient and C_i inter-cellular CO_2 concentrations, D is vapor pressure deficit between leaf and atmosphere (in terms of water-vapor concentrations, e_i and e_a) and a is the ratio of H_2O stomatal conductance to CO_2 stomatal conductance ($a = 1.6$).

Leaf energy balance

The net energy per unit leaf area, Δ , on a particular canopy layer, z , can be balanced as

$$\Delta = \Theta_z - H - LE \quad (9)$$

where, Θ_z is the solar radiation flux falling on that canopy layer, H is rate of heat lost (or gained) from the leaf to the ambience due to convection, LE is the rate of latent heat lost from leaf due to transpiration from stomatal pores. Heat lost through radiation is neglected. In terms of temperatures Eq. (9) can be expanded for *non-steady* states; as

$$\frac{dT_l}{dt} = \frac{1}{m_{l,w} C_{pl}} [\Theta_z - \rho_a C_{pa} (T_l - T_a) g_h - ag_s D \times LE] \quad (10)$$

where T_a and T_l are temperatures of ambient air and leaf surface respectively, $m_{l,w}$ is wet mass of total leaves per unit area of that canopy layer and ρ_a is density of air at T_a , C_{pl} and C_{pa} are specific heat capacities of leaf and air respectively and g_h is heat conductance as derived in Eq. (6).

Eq. (10) is discretized with finite difference scheme and solved for T_l with *Runge-Kutta* method. Initial vertical profile of T_l i.e. T_l^0 is required to march the solution scheme with respect to time.

Leaf biochemical reactions

The temperature dependent photosynthetic kinetics are fundamentally developed by Farquhar et al (1980), which are adapted in this model. The expression for the flux of CO_2 released, f_c is,

$$f_c = \frac{a_1 (C_i - C_p)}{a_2 + C_i} \quad (11)$$

where C_p is CO_2 compensation point, a_1 and a_2 are selected constants depending on whether the photosynthetic rate is *light* or *Rubisco* limited. Under light saturation conditions, $a_1 = V_{cmax}$ (maximum carboxylation capacity) and $a_2 = K_c (1 + C_{oa}/K_o)$, where K_c and K_o are the *Michaelis constants* for CO_2 fixation and oxygen inhibition

and C_{oa} is the oxygen concentration in air. The temperature dependent bio-chemical reaction parameters and rate constants are dependent on leaf temperature, T_l . The temperature correction of various leaf parameters is provided in Table 1 (adapted from Katul et al 2000).

Stomatal optimization

The stomatal regulation is crux of the tree behavior. There exists an ambiguity in quantifying the interplay of stomatal regulation when it tries to economize the trade-offs between loss of water and gain of carbon. The trouble inherent in quantifying the of role of stomatal conductance is due to its dependence on multiple feed-back signals. However, Katul et al (2010) have come up with a calculus based analytical model for stomatal conductance which is based on *Fickian* mass transfer of CO_2 and H_2O through stomata. Their objective is to frame an optimization problem with a goal to maximize the carbon gains at the cost of transpiration. Even though their work is not directly related to SPAC, it provides valuable insight into the dynamic behavior of stomata with respect to the instantaneous micro-climatic variables existing at that canopy layer. Further, they have arrived at a semi-constant, λ called marginal water use efficiency (carbon budget equivalence), which converts the transpiration losses into the carbon budget equivalence. The stress condition in the vegetation can be reflected into the model with higher values of λ . The calculus based approach to determine the stomatal conductance (Katul et al 2010) is computationally inexpensive and quicker in comparison to the iteration based approach by Williams et al (1996).

The value of stomatal conductance, g_s in Eq. (12) for which $f(g_s)$ turns out to be minimum; i.e. at the optimum stomatal conductance (Givnish and Vermeij 1976).

Table 1 Biochemical parameters and their temperature adjustments for Eq. (11), adapted from Katul et al (2000)

Parameter	Value or temp. adjustment	Units
V_{cmax}	59	$\mu\text{mol}/\text{m}^2/\text{s}$
$K_{c,25}$	300	$\mu\text{mol}/\text{mol}$
$K_{o,25}$	300	$\mu\text{mol}/\text{mol}$
$C_{o,a}$	210	$\mu\text{mol}/\text{mol}$
C_p	$36.9 + 1.18(T_l - 25) + 0.036(T_l - 25)^2$	$\mu\text{mol}/\text{mol}$
a_1 (i.e. V_{cmax})	$V_{cmax,25} \frac{\exp[0.88(T_l - 25)]}{1 + \exp[0.29(T_l - 41)]}$	$\mu\text{mol}/\text{m}^2/\text{s}$
K_c	$K_{c,25} \exp[0.074(T_l - 25)]$	$\mu\text{mol}/\text{mol}$
K_o	$K_{o,25} \exp[0.015(T_l - 25)]$	$\mu\text{mol}/\text{mol}$
a_2	$K_c \left(1 + \frac{C_{oa}}{K_o}\right)$	$\mu\text{mol}/\text{mol}$

Analytical expression for final value of g_s , after differentiating Eq. (12) with respect to g_s ,

$$f(g_s) = f_c - \lambda f_e \quad (12)$$

$$\begin{aligned} \frac{\partial f(g_s)}{\partial g_s} &= 0 \\ g_s &= \frac{-a_1(a_2 - C_a + 2C_p)}{(a_2 + C_a)^2} \\ &+ \frac{\sqrt{aD\lambda a_1^2(C_a - C_p)(a_2 + C_p)(a_2 + C_a - 2aD\lambda)^2(a_2 + C_a - aD\lambda)}}{aD\lambda(a_2 + C_a)^2(a_2 + C_a - aD\lambda)}. \end{aligned} \quad (13)$$

and involving substitutions from Eqs. (7), (8), and (11) can be derived as Eq. (13) (Katul et al 2010). Where λ is carbon budget equivalence, a semi-constant parameter which necessarily equates the amount of water transpired, f_e , in terms of carbon spent on it, f_c .

The expression for optimal stomatal conductance, g_s , in Eq. (13) is substituted in energy balance statement of Eq. (10). The water-vapor concentration differences, D , between inter-cellular leaf spaces and ambient air is one of the regulating signals in determining the stomatal conductance [Eq. (13)], as well as leaf temperature [Eq. (10)], further, it is directly dependent on leaf temperature, T_l . Assuming ideal gas equivalence to water-vapor; both in leaf spaces and in ambient air, the difference in molar concentrations, D , can be expressed as

$$D = e_i - e_a = \frac{P_l}{RT_l} - \frac{P_a}{RT_a} \quad (14)$$

where P_l and P_a are saturated water-vapor pressure inside the leaf spaces and water-vapor pressure in ambient air respectively (Appendix B), R is ideal gas constant. It is to be noted that, water-vapor concentrations inside the leaf spaces are reasonably assumed at saturation conditions at T_l , whereas vapor concentrations in ambient air are derived from measured data of relative humidity, RH_a levels at that ambient temperature, T_a .

In order to find out the evaporation losses, f_e , from the leaf surface, the explicit expression for stomatal conductance from Eq. (13) is substituted in Eq. (8). Further, the explicit expression for CO_2 flux, as derived by Katul et al (2010) is

$$\begin{aligned} f_c &= \frac{1}{2}(a_1 + (a_2 + C_a)g_s) \\ &- \sqrt{[a_1 + g_s(a_2 - C_a)]^2 + 4g_s(a_1C_p + a_2C_ag_s)}. \end{aligned} \quad (15)$$

Flow of water

Flow of water in the trees is explained with Cohesion theory of sap ascent. The loss of water from the leaves,

f_e , causes a fall in leaf water potential, ψ_{leaf} , setting up a gradient of potential from leaves to the roots. Necessarily, the water up-taken by the roots is to be transmitted through the stem to the various canopy layers, therefore a balance of water can be setup in stem section, where input rate (root uptake) of water is equal to the output rate (transpiration). The water storage component of trees and the hydraulics of stem is not considered at this stage of model development. The root-water uptake is primarily governed by the negative water pressure head, ψ_{stem} , developed at the stem section, which is due to a result of cumulative, ψ_{leaf} , developed across multiple canopy layers.

The flow-diagram of the proposed model is shown in Fig. 3. In each time step the model finds out suitable value of ψ_{stem} ($\leq \psi_{stem, minimum}$, which is the minimum negative pressure head the tree can sustain), which would necessarily picks up the equivalent amount of water from soil in order to balance the transpiration demand. As there is no closure relation to quantify the value of ψ_{stem} , the relation is established iteratively.

Fig. 3 Flow diagram of the developed model

Root water-uptake

Typically the water movement in soil layers is treated as the one-dimension vertical flow in an unsaturated medium. This process is mathematically modeled by the celebrated Richards equation, which is an integrated form of *Darcy's equation* of water volume flux and the *Continuity equation*. In most of the models, the water uptake by roots is represented by a volumetric sink term (macro-scale approximation) in Richards equation. It involves the information about the roots as functions of; root density, root axial and radial water conductivities, equivalent root diameter and time varying water pressure profiles along the depth of roots.

Richards equation

The Richards equation for isotropic medium in vertical dimension can be written as:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right] - F(h) \quad (16)$$

where C is the differential water capacity ($C(h) = \frac{d\theta(h)}{dh}$, θ is water capacity), h is soil water pressure head, t is the time, K is the unsaturated hydraulic conductivity, z is the vertical coordinate (positive upward), and F is the root water extraction. Both finite difference and finite element methods are used to solve Eq. (16). Finite elements are advantageous at irregular geometry in two and three-dimensional flow domains. In one-dimension finite difference is advantageous because it needs no mass lumping to prevent oscillations and is relatively easy to conceive and to implement in numerical routines.

The Eq. (16) requires two boundary conditions of *Newman* type, one is Q_{top} , evaporation or precipitation flux on top soil layer and the second is Q_{bot} , seepage flux of water into the underneath soil layers. Initial soil-water pressure head profile, h_i^0 , is also necessary to initiate the root-water uptake module.

van Genuchten and Mualem relations

The relationships between *soil saturation and soil-water pressure head*; and between *soil hydraulic conductivity and saturation* are adapted from the van Genuchten and Mualem equations. The former can be shown as

$$S(h) = \begin{cases} (1 + |\alpha_v h|^{n_v})^{-m_v} & h < 0 \\ 1 & h \geq 0 \end{cases} \quad (17)$$

and the later

$$K(h) = K_s S(h)^{1/2} \left[1 - \left(1 - S(h)^{1/m_v} \right)^{m_v} \right]^2 \quad (18)$$

where S is effective saturation as a function of soil-water pressure head, K_s is saturation soil water conductivity (van

Genuchten 1980), α_v is a parameter used to scale the soil matric pressure head and m_v is a dimensionless parameter related to the width of the pore size distribution. The $S(h)$ terms in Eq. (18) is substituted by Eq. (17) to get conductivity $K(h)$ as solely dependent on h . Further

$$C(h) = \frac{d}{dh} (\theta(h)) \quad (19)$$

is obtained by differentiating $\theta(h)$ term with respect to soil water pressure head. The relation involving residual and saturated water capacities

$$\theta(h) = \theta_r + (\theta_s - \theta_r) S(h) \quad (20)$$

is substituted into Eq. (19), the final expression for differential water capacity would look like

$$C(h) = (\theta_s - \theta_r) \left[-m_v (1 + |\alpha_v h|^{n_v})^{-m_v-1} \right] [n_v |\alpha_v h|^{n_v-1} \alpha_v]. \quad (21)$$

Finally Eqs. (18) and (21) are substituted into Eq. (16) and discretized accordingly.

Sink

The sink term in Eq. (16) is only through the depth-wise water uptake by roots. The tree root system can be approximated into a zero ordered cylindrical equivalence or 1st ordered equivalent cylindrical root with branched cylinders protruding out at regular intervals. For simplicity zero ordered root equivalence is assumed. The mass conservation principle for water (incompressible) is applied over the system of soil and roots. The root system of trees are represented with an equivalent cylindrical hollow tube. Nevertheless, there exists a scope to accommodate the complex geometry of root system accordingly. For the assumption made in this model, the continuity equation would look like Eq. (22) (adapted from Roose and Fowler 2004), which is derived by balancing the radial incoming flux of water into the root and the upward axial movement of water,

$$2\pi a k_r (p_s - p_r) = -k_z \left(\frac{\partial^2 p_r}{\partial z^2} \right), \quad (22)$$

where p_r is root water pressure, p_s is soil water pressure as a function of depth z , a is equivalent cylindrical root radius, k_r is root radial conductivity coefficient, and k_z is root axial conductivity coefficient.

The Eq. (22) is solved with bottom boundary condition

$$\frac{\partial p_r}{\partial z} - \rho g = 0$$

at $z = L$ (end of cylindrical root) because of the structural properties of the root-tip which precludes the water flux, where ρ is density of water and g is acceleration due to

gravity. The boundary condition at the top of the cylindrical root is

$$p_r = \psi_{stem}$$

at $z = 0$, where ψ_{stem} is the *driving pressure* at the base of the stem (or beginning of root structure); just at the ground level, which governs the amount of water to be up-taken from the soil layers.

Discretization

Eq. (16) is solved by finite-difference scheme adapted from Belmans et al (1983) and van Dam and Feddes (2000), which is implicit and applies an explicit linearization of $K(h)$ and $C(h)$ terms. The discretized Eq. (23) is valid for all nodes except for top and bottom (within the unsaturated zone) at which the boundary conditions are accounted. Notation j is in the direction of time, t , and i along the depth, z , with fixed (or varying) time step Δt and spatial step size Δz .

$$\frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{K_{i-\frac{1}{2}}^j \left(\frac{\Delta h_{i-\frac{1}{2}}^{j+1}}{\Delta z} + 1 \right) - K_{i+\frac{1}{2}}^j \left(\frac{\Delta h_{i+\frac{1}{2}}^{j+1}}{\Delta z} + 1 \right)}{C_i^j \Delta z} - \frac{F_i^j}{C_i^j} \quad (23)$$

here $K_{i-\frac{1}{2}}^j = (K_i^j K_{i-1}^j)^{\frac{1}{2}}$ and similarly for $K_{i+\frac{1}{2}}^j = (K_i^j K_{i+1}^j)^{\frac{1}{2}}$ as suggested by Vauclin et al (1979). Further Eq. (22) is simply discretized as

$$2\pi a k_r (p_{s,i}^j - p_{r,i}^j) = -k_z \frac{(p_{r,i+1}^j - 2p_{r,i}^j + p_{r,i-1}^j)}{(\Delta z)^2} \quad (24)$$

where $p_{s,i}^j$ is nothing but h_i^j term, where the former is in pressure units and the later is in pressure head units. Eqs. (23) and (24) are solved in couple to obtain the vertical profiles of $p_{s,i}^j$ and $p_{r,i}^j$. F_i^j can be calculated from the following expression,

$$F_i^j = 2\pi a k_r l_d t (p_{s,i}^j - p_{r,i}^j)$$

where l_d is root density. Physically, the soil water pressure influences the profile of water uptake according to the corresponding root water pressure profiles, change in one would reflect in others and vis a vis. The water uptaken from the soil matrix will be balanced with cumulative transpiration losses at that time step,

$$\sum F_i^j = \sum f_e$$

from all the canopy layers.

Model implementation

Various modules mentioned in the flow diagram are coded in *GNU Octave* programming language (Eaton 2002), which are all discretized and coupled internally to represent the non-steady state behavior and dynamism. The model output graphs are drawn in R statistics (R Development Core Team 2008).

In the present paper, the framework of proposed model is alone discussed, the validation of the model with field data is being studied and will be presented subsequently. In order to appreciate the dynamic behavior of the model, the model is run for 24 h duration with the required inputs. The soil and vegetation related variables (and parameters) are chosen apparently from the CSIR—National Environmental Engineering Research Institute campus and micro-climatic variables are measured with the weather station.

Study area

The study area is located in an urban forest area of CSIR—NEERI campus, in Nagpur city of Central India ($21^\circ 7' 14'' \text{N}$, $79^\circ 4' 19'' \text{E}$, mean sea level + 315.0 m), which falls under dry tropical climate region with clayey soils. The forest stand is approximately 50 years old, primarily consisting of *Leucaena leucocephala* trees. Canopy of the stand appears to be sparse, permitting enough solar radiation to reach the lengths of individual trees.

Data

Diurnal wind speed, U_{top} , ambient relative humidity, RH_a and ambient air temperature, T_a measured by weather station are fed into the model (shown in Fig. 4a, b) in real time, based on the time step of the model, Δt . Solar irradiance data is simulated by Eq. (2) (shown in Fig. 4c). Ambient atmospheric CO_2 concentration, C_a , is measured by Open-path infrared gas analyzer. Soil top and bottom layer water fluxes Q_{top} and Q_{bot} are fed as boundary conditions, whereas, T_l^0 , initial leaf temperature profile as initial condition. Apparent properties of the vegetation and soil are presented in Tables 2 and 3. The constants used in the model is presented in Table 4.

It is found that the subtle changes in stomatal conductance can be recognized at half hour intervals, hence temporal resolution is fixed at 30 min, otherwise it can be any value depending upon the availability of data frequency. Spatial resolution of 0.1 m is chosen for vadose zone and 0.5 m for canopy layers (Table 5).

Fig. 4 30 min averaged input data for 24 h. **a** Wind-speed. **b** Relative humidity and ambient temperature. **c** Hourly global solar radiation. Model outputs. **d** 30 min averaged stomatal conductance. **e** Soil

depth-wise profile of soil-water pressure head with respect to time, in order to satisfy the cumulative transpiration demand of $F_w = 46 \text{ l/m}^2/\text{d}$

Results and discussions

The model simulates the dynamic stomatal conductance, g_s , values based on the input data of 24 h cycle, which would determine the transpiration losses, and thus effects the water uptake pattern and soil moisture content along the depth of soil (shown in Fig. 4d). It is estimated that with the given data, the trees would transpire 46 liters of water per unit area of canopy per day ($F_w = 46 \text{ l/m}^2/\text{d}$).

Due to the uptake of $46 \text{ l/m}^2/\text{d}$ of water from the soil, the profile of soil-water pressure head over the depth, keeps on changing with respect to time (shown in Fig. 4e). The variation in the profiles is conspicuous at the root depth of 1 m, as the roots play a key role in influencing the soil moisture content. Further, due to continuous water uptake, the initial soil pressure head profile ($h_i^0 = -100 \text{ cm}$) kept on shifting in the direction of negative pressure, by following the boundary conditions of $Q_{top} = 0$ and

Table 2 Vegetation properties of *Leucaena leucocephala* used in the model

Parameter	Value	Unit
Root depth, L	1.0	m
Avg. root density (cylindrical approx.), l_d	1	m/m ³
Root axial conductivity, k_a	1.198×10^{-6}	m ⁴ /s/MPa
Radial conductivity, k_r	2.49×10^{-5}	m/s/MPa
Radius of root, r	0.15	m
Initial leaf temperature, T_l^0	25	⁰ C
Specific heat capacity of leaf, C_{pl}	3750	J/Kg/K
Effective leaf length, l_e	0.26	m
Top height of canopy, H_t	10	m
Bottom height of canopy, H_b	3	m
λ	700	–
LAI	2.3	–

Table 3 Soil properties used in the model

Variable/parameters	Value	Unit
Soil top-layer water flux, Q_{top}	0.0	cm/d
Bottom layer water flux, Q_{bot}	1.8	cm/d
Initial soil water pressure head, h_i^0	–100	cm
Residual soil water content, θ_r	0.1	cm ³ /cm ³
Saturation soil water content, θ_s	0.5	cm ³ /cm ³
α_v	0.011	–
n_v	2.5	–
Soil saturation conductivity, K_s	20	cm/d

Table 4 Constants used in the model

Parameter/constant/variable	Value	Unit
Density of air, ρ_a	1.204	Kg/m ³
Specific heat capacity of air, C_{pa}	1004	J/Kg/K
Thermal diffusivity in air at 300 K, D_h	1.9×10^{-5}	m ² /s
Density of water, ρ	1000	Kg/m ³
Acceleration due to gravity, g	9.81	m/s ²

Table 5 Spatial and temporal resolution of the model

Variable	Value	Unit
Time step, Δt	30	min
Step size along the depth of soil, Δz	0.1	m
Step size along the depth of canopy	0.5	m

$Q_{bot} = 1.8$ cm/d. It is also seen that, the pressure head profile at $t = 24$ h has shifted towards the positive pressure head direction, which can be due to the regaining of moisture ($Q_{bot} = 1.8$ cm/d, bottom boundary condition) in non-transpiring hours.

The distribution of H₂O fluxes (transpiration losses) over the depth of canopy layers is shown in Fig. 5. As

Fig. 5 Breakup of cumulative canopy transpiration loss, $F_w = 46$ l/m²/d over the depth of canopy

various canopy layers receive different weather conditions viz. solar-radiation and wind-speed (which is due to the distribution of LAI), the water demand from each canopy layer is different. The top layers transpire more amount of water in comparison with the bottom layers, as they experience higher leaf temperatures due to higher solar radiance and also experiences the higher wind-speed.

Climate change scenarios

Hypothetical climate change scenarios are performed on the model in order to quantify the changes in tree water-uptake pattern due to increase in wind speed, U_{top} , relative

Fig. 6 Changes in transpiration pattern, due to **a** increase in wind-speed, **b** increase in ambient CO₂ concentration C_a , **c** simultaneous increase in ambient air temperature T_a and C_a , and **d** simultaneous

increase in relative humidity RH_a and T_a . While the variables are varied, the rest of the model inputs are kept as constants

humidity, RH_a , ambient CO₂ concentration, C_a and ambient air temperature, T_a . The values of these weather variables are selectively hiked (over the 24 h cycle data fed into the model, Fig. 4a–c) by keeping the rest of variables as constants. For an increase of wind-speed from 0 to 5 m/s over the input diurnal wind profile, the model estimated a marginal rise in cumulative transpiration demand from 46 to 46.12 l/m²/d (Fig. 6a). Higher wind-speed causes the decrease in leaf boundary layer thickness, hence favors transpiration.

It is observed that there is a decrease in transpiration rate from 46 to 34 l/m²/d (shown in Fig. 6b) due to the increase in ambient CO₂ concentration, C_a from 600 to 800 mmol/m³. This behavior is also supported by Carlson et al (1980) and Katul et al (2010), further Katul et al (2010)

hypothesized that due to the reduction in transpiration from the leaves, the soils will remain with sufficient moisture, hence amplifies the surface-runoff process, leading to the leaching problems.

The effect on transpiration losses due to the simultaneous variations of increased ambient air temperature, T_a from 0 to 5 °C and increased ambient concentration of CO₂, C_a from 600 to 800 mmol/m³ is tested by the model. The model estimated a slight decrease in transpiration demand from 46 to 41.37 l/m²/d (surface plot of Fig. 6c), which is due to the result of both negative and positive feed-backs by C_a and T_a respectively.

Similarly, another hypothetical situation is tested by the model (Fig. 6d), in which the relative humidity, RH_a is increased from 0 to 20 %, and ambient air temperature, T_a

Fig. 7 Increase in transpiration losses with decrease in leaf size (at constant existing environmental variables)

from 0 to 5 °C. The model estimated a slight decrease in transpiration demand from 46 to 42.52 l/m²/d, due to the interaction of both negative and positive feed-backs by RH_a and T_a . Rawson et al (1977) experiments confirms the decrease in transpiration due to higher relative humidity or lower vapor-pressure-deficit.

Further, the model helps in verifying some of the evolutionary traits of species in terms of its leaf size and shape. For instance, the leaf size of a particular species is adjusted to the existing environmental situations; in order to optimize its energy consumption so as to reduce the water lost for the assimilation of carbon. The model estimates that, due to the increase in the effective leaf length, l_e there is a subtle decrease in transpiration losses (Fig. 7). This behavior is explained with the increased thickness of leaf boundary layer with the increase of l_e , thus decreases the leaf boundary layer conductance. The model predictions can potentially throw some light in explaining the differences in leaf size and shape of trees from same climatic zones.

Conclusions

The philosophy behind this modeling framework is to consider the tree as a living entity, which continuously interacts with the surrounding environmental variables so as to behave in terms of water uptake. The proposed modeling framework can be appreciated as a research tool to comprehend the enormity of processes occurring in the

Soil-Tree system. The model can be useful in hypothesis testing and resource optimization in the light of various climate change scenarios. Also the model can be integrated with remote-sensing data in order to estimate the regional-scale spatial patterns of water-uptake by vegetation.

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Appendix A: A radiation regime

1. $W_s = \cos(-\tan(\phi)\tan(\delta))$, ϕ is latitude of the location (degrees), δ is declination angle of sun (degrees).
2. $\delta = 23.45 \times \sin\left(360 \times \frac{284 + \text{day}}{365}\right)$.
3. $W = \frac{360}{24}(h - 12)$, h is the time of the day (solar time in hours).
4. $a = 0.409 + 0.5016 \times \sin(W_s - 60)$.
5. $b = 0.6609 + 0.7467 \times \sin(W_s - 60)$.

Appendix B: Saturated water vapor pressure

1. Saturated vapor-pressure inside the leaf.

$$P_l = 6.11 \times \exp\left[\frac{17.27 \times T_l}{T_l + 237.31}\right]$$

2. Vapor-pressure in ambient air.

$$P_a = \frac{RH_a}{100} \times 6.11 \times \exp\left[\frac{17.27 \times T_a}{T_a + 237.31}\right]$$

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