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# Control of atmospheric fluxes from a pecan orchard by physiology, meteorology, and canopy structure: Modeling and measurement

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#### ABSTRACT

We constructed and validated against eddy-covariance data a model of the fluxes of water vapor, sensible heat, CO<sub>2</sub>, and radiation in a substantially mature pecan orchard (*Carya illinoinensis* (Wangenh.)K. Koch) in an arid environment near El Paso, TX, USA. The detailed process-based model is designed for insights into major control points for photosynthetic gain and water use as exerted by canopy structure, leaf physiology, and micrometeorological drivers. Toward this end, it resolves extensive details of leaf micro environments (radiation and scalars) in realistic canopy structures, as well as photosynthetic and respiratory physiology, stomatal control, and water relations from roots to leaves. The model is for a static mid-season canopy, with the ability to link it to dynamics models of development and management. Field flux measurements agreed well with model estimates that were derived using measurable parameters rather than data-fitting. An exception was the measurement-model disparity in sensible heat flux under conditions of strong advection of dry air; the model diagnostics imply a marked insensitivity of pecan stomata to humidity that has not been reported earlier. Formulation and parametrization of most of the physical and physiological processes was robust, shared well between the study site and an alternate site, but gaps are evident in the knowledge of several important processes, primarily in responses to water stress. The study indicates limitations in simpler models, such as those based on constant canopy conductance or light-use efficiency, while offering leads to making more accurate simple models suitable for use in decision support systems, ultimately for stress management under limited water availability. © 2013 Elsevier B.V. All rights reserved.

#### 1. Introduction

Agricultural water management faces challenges at multiple scales, from growers to water authorities. On a global scale, irrigation shortfalls are expected to increase (Wada et al., 2012), with water shortages extending to other, competing consumptive uses (Vörösmarty et al., 2010). Some of the challenges may be addressed with optimal irrigation methods on farms and in orchards. Irrigation scheduling to avoid stress (e.g., Miyamoto, 1984; Kallestad et al., 2006) is one element. Optimization of stress levels to limit yield reductions and improve water-use efficiency is another element, having been explored primarily under the rubric of deficit irrigation (DI; Behboudian and Mills, 1997) and related but not equivalent partial root drying (Fernandez et al., 2006; Romero et al., 2005). For tree nut crops such as we focus upon, DI has been studied (pistachio, *Pistacia vera* L: Gijon et al., 2009; Goldhamer and Fereres, 2004; Romero et al., 2005; Shackel et al., 2000). However,

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the detailed physiological basis of stress responses has not been elucidated; experiments remain empirical, with intuition dominating over physiological process knowledge. Process-based models afford the opportunity to integrate extant knowledge while highlighting the limitations of such knowledge for productive research direction. Provided that the known processes are formulated with robust models, model simulations enable the identification of a small suite of most informative experiments, reducing the research effort. By "robust models," we mean models that have been comprehensively tested and that have ready or, best of all, nearly universal parameterization, such as the photosynthesis model of Farquhar et al. (1980). Such reduction of the scope of experiments is particularly merited in studies of stress. Long-lived woody crops are valuable, and growers rarely are willing to risk their investment on experiments, and then only with a deep justification. Once tested, process-based models also can be applied in new locations and climates with notably better confidence than with empirical or statistical models.

Of course, complex process-based models must be reduced to simpler models for application by farmers, growers, and water managers. A simpler model is then profitably incorporated into a user-friendly interface that allows the specification of management

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options. The resultant decision support system (DSS) must also provide predicted results such as yield in a compact, comprehensible manner. It is also valuable for the DSS to provide key diagnostics of intermediate results (water status, etc.) that can be checked in the field. Making a useful DSS is fraught with pitfalls (Matthews et al., 2008), as is even the development of the complex base model (Johnson, 2011; Vogel et al., 1995), but a great variety of DSSs have been developed; a search on "decision support system" "agriculture" returned 174 results. For example, the DSSs for soybean (*Glycine max* (L.) Merr.) (SOYGRO; original reference Wilkerson et al., 1983) and cotton (*Gossypium hirsutum* L.) (GOSSYM; original reference Fye et al., 1981) have been used for many years.

The trajectory of developing a comprehensive model, then simpler models that are locally parametrized, and finally a DSS, is mandated not by computational demand but by the need to reduce "data hunger" for the ultimate users. Current levels of computational power and of mathematical methods make the execution of extremely large models practical on short time scales. However, complex agricultural models generally involve specification of many parameters for crop physiology, soil properties, and crop structure, - more than growers and farmers can afford to measure as model inputs. DSS developers then bear the burden of projecting complex models to simpler forms. In this task, they can apply knowledge of the patterns of parameters over wide geographic regions, climates, soils, and crop varieties. More to the point of the current effort, the developers can identify robust process descriptions to use in simpler models. We have cited above the photosynthesis model of Farquhar et al. (1980), and there is evidence that stomatal control models originating with the model of Ball et al. (1987) are robust. Using complex models such as we present here can aid in discovering more such robust descriptions. Another utility of complex models is discovering the parameters to which crop performance is most sensitive, thus, the parameters for which accurate measurement is most necessary.

The current study presents a model for whole-orchard energy fluxes and photosynthesis, as well as the justifications for decisions on its structure. The model is intended to be a major step in developing a decision support system, as well as to aid the development of better crop models of diverse physiological, biophysical, and meteorological processes at suitable levels of detail for each process. It will be incorporated into a larger modeling framework, comparable to that presented in previous work (Andales et al., 2006). The simulations are tested against flux measurements by eddy covariance, as well as for internal consistency.

#### 2. Materials and methods

#### 2.1. The model

#### 2.1.1. Basic structure

The model computes and sums fluxes of water vapor, heat, and  $CO_2$  on an hourly basis from individual leaves, sampled at a selectable number of locations within the crown of a central tree as steps in radius, zenith, and azimuth. Leaves are also sampled at a finite number of angular orientations. A uniform leaf angle distribution in zenith and azimuth is assumed (Ross, 1981). A user of the model specifies orchard structure that affects light interception, specifying for the central tree and an arbitrary number of neighboring trees in rows and columns each tree's location (centroid Cartesian coordinates) and its crown geometry as an ellipsoid of revolution (major and minor axis dimensions and zenith and azimuthal angles of the major axis tilt). All crowns are modeled as having a uniform foliage density,  $f_d$ , throughout their volume. The fluxes of water vapor, heat, and  $CO_2$  at a central tree are taken as representative of the whole orchard, and they are subsequently scaled to fluxes per unit ground area for comparison with eddycovariance data. The parameters and variables in the model are summarized in Table 1.

The model currently does not resolve latent and sensible heat fluxes at the soil, canopy rainfall interception or dewfall, or transients in photosynthetic fluxes from varying light levels. The model uses a static canopy structure as a useful approximation for important midseason performance.

The model is coded in Fortran 90 with extensive commenting. Variables are all of explicitly declared type, with descriptions of their meaning and their physical units. The code and sample input data and output files are available online at http://gcconsortium. com/pecan/pecan\_model.pdf and at http://pecanmodel.blogspot. com/p/model-version-2012-05-14.html.

#### 2.1.2. Leaf properties and processes

Leaf linear dimension,  $d_{\text{leaf}}$ , crosswise to the midrib, is specified for computing the convective heat transfer. Leaves are described, first, by their optical properties (absorbances in the wavebands of photosynthetically active radiation [PAR] and near-infrared radiation [NIR] and corresponding transmittances). Second, their photosynthetic physiology is described within the robust model of Farquhar et al. (1980), by: maximal carboxylation capacity (V<sub>c,max</sub><sup>25</sup>, light- and CO<sub>2</sub>-saturated); CO<sub>2</sub> and O<sub>2</sub> binding constants  $K_{\rm C}$  and  $K_{\rm O}$ ; photorespiratory offset  $\Gamma^*$ ; initial quantum yield at CO<sub>2</sub>saturation  $Q_0$ ; the transition parameter  $\theta_{PS}$  between light-limited and light-saturated regimes; and the standard temperature dependences of these quantities. Photosynthetic limitations posed by electron transport or triose-phosphate transport are not accounted, as they are commonly significant only at elevated CO<sub>2</sub> levels. Employing a simplification (linearization) of the empirical studies of Niinemets (2007), maximal photosynthetic capacity is modeled as linearly proportional to mean PAR irradiance at each canopy location, with a nonzero intercept (Lombardini et al., 2009). The mean PAR irradiance is evaluated on a user-specified day, chosen as typical of the season. Third, the leaf basal respiration rate is specified at the mean photoperiod temperature,  $T_{mean}$ , of the preceding two weeks, to which this respiration has acclimated (Wythers et al., 2005). Respiration at other temperatures is scaled by the factor  $exp(0.07^*[T_{leaf}-T_{mean}])$ , where  $T_{leaf}$  is the leaf temperature). The basal leaf respiration rate is scaled at each canopy location as directly proportional to the value of photosynthetic capacity at that location. The stomatal control program is formulated in standard Ball-Berry form (Ball et al., 1987) for stomatal conductance,  $g_s = m_{BB}A h_s/C_s + b_{BB}$ . Here, the slope,  $m_{BB}$ , and the intercept,  $b_{BB}$ , are fixed parameters, A is the leaf photosynthetic rate, and  $h_s$ and C<sub>s</sub>, are relative humidity and CO<sub>2</sub> mixing ratio at the leaf surface. Two options switches described in the Results and Discussion allow the user to apply an exponent other than unity to the surface relative humidity,  $h_s$ , and to use either net or gross leaf photosynthesis. Newer alternative formulations (Leuning, 1995; Dewar, 2002) were found to give slightly poorer fits to leaf gas-exchange data on other pecan trees (Johnson, 2004).

#### 2.1.3. Projection of microenvironment to the leaf level

Weather data are taken from a weather station location 1.2 km to the southeast of the eddy-covariance tower. Humidity and temperature within the canopy are taken as uniform at all leaves, as in common two-layer models, while being modified from free-air values by canopy self-humidification and self-heating. Consequently, water vapor pressure in the air within the canopy,  $e_{air,can}$ , is modeled as  $e_{air,can} = e_{air} + E P_{air} r_a = e_{air} + E P_{air}/g_a$ , where:  $e_{air}$  (in *Pa*) is the free-air value at the weather station; *E* is the transpiration flux density per unit ground area in units of mol m<sup>-2</sup> s<sup>-1</sup>;  $P_{air}$  is total air pressure in *Pa*; and  $r_a$  is the canopy aerodynamic resistance,  $1/g_a$ , also in molar units. The value of aerodynamic conductance,  $g_a$  (in

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