EVALUATING SIMPLE TRANSPIRATION–BASED MODELS OF CROP

PRODUCTIVITY

By

CRISTIAN KREMER

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To the Faculty of Washington State University:

The members of the Committee appointed to examine the dissertation of CRISTIAN KREMER find it satisfactory and recommend that it be accepted.

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Chair

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EVALUATING SIMPLE TRANSPIRATION–BASED MODELS OF CROP PRODUCTIVITY

Abstract

by Cristian Kremer, Ph.D.
Washington State University
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Chair: Claudio O. Stöckle

There is a renewed interest in evaluating crop productivity using simple transpiration–based models of biomass accumulation. Transpiration–use efficiency (w), defined as the ratio of biomass (B) produced per unit water transpired (T), has been widely used to evaluate crop performance under limited water supply. Simple approaches to asses w have been used including: 1) $w = k_{Da}/D_a$ and 2) $w = k_{ETo}/ET_o$; where k_{Da} and k_{ETo} are crop-dependent parameters. The concept is that normalization by D_a or ET_o would account for the effects of climate variations on w, while k_{Da} or k_{ETo} would be reasonably constant across diverse environments. However, the evaluation of the transferability of these parameters is not simple due to the scarcity of experimental values and the lack of consistency of the methodology used in the available experiments. For this reason we have developed and tested a canopy transpiration and photosynthesis model (CTP) to obtain simulated values of w, k_{Da} and k_{ETo} in different locations with a consistent methodology. Model simulations were compared with evapotranspiration estimated with weighing lysimeters for non stressed wheat and maize. Results showed good agreement between observed and simulated transpiration values for both crops, with the simulated values tracking well the daily fluctuations of the observed values. Daily values of simulated transpiration–use efficiency (w) were compared with observed values

from literature and showed that the average and standard deviation of the simulated values were within the range of the observed data. The model was then used to evaluate the transferability of k_{Da} and k_{ETo} values for wheat and maize across eight world locations with contrasting climate. The results indicated that k_{Da} and k_{ETo} (maize) are not constant parameters; suggesting that calibration in contrasting climates would be desirable. However, a consistent trend of change of the values of these parameters as a function of D_a or ET_o was found, which can be represented by mathematical functions, allowing the possibility of transferring k_{Da} and k_{ETo} values across climatic conditions. Verification of these equations with field data was performed. The simulation–based equations to estimate w and k_{Da} of wheat and maize, and k_{ETo} of maize appeared to be robust estimators of observed values, while k_{ETo} of wheat was better represented by a single value across climatic conditions.

EXECUTIVE SUMMARY

An increasing need to evaluate crop productivity under limited or uncertain water supply scenarios has renewed interest in simple, transpiration–based models of crop productivity that can be readily applied to a large number of crop species across the entire range of climatic conditions where these crops are grown. Simple approaches to asses transpiration–use efficiency (w), defined as the ratio of biomass produced per unit of water transpired, has been used to evaluate crop productivity as a function of water supply including : 1) $w = k_{Da}/D_a$ (Bierhuizen and Slatyer, 1965; Tanner and Sinclair, 1983), and 2) $w = k_{ETo}/ET_o$ (Steduto and Albrizio, 2005); where k_{Da} and k_{ETo} are crop–dependent parameters. Normalization by D_a or ET_o should account for the effects of climate variations on w, while k_{Da} or k_{ETo} are expected to be reasonably constant across diverse climatic conditions. However the experimental determination of the parameters used in the models has been relatively scarce, partially due to the need of measuring crop transpiration for their determination. In addition, the experimental data has focused only on a few crops and is largely insufficient.

As a result of the scarcity of experimental information, it is not easy to assess the variability and transferability among locations of the parameters. The problem is compounded because a fraction of the variability can be traced back to the use of different crop varieties, crop management, methods of determination of transpiration rates, methods for biomass sampling, and plain experimental error.

The development of a detailed mechanistic model of canopy transpiration and photosynthesis, which can be utilized as a tool to simulate the parameters of simple transpiration–based models, is a useful approach to evaluate the transferability of these

parameters across diverse climatic conditions without the shortcomings of the available experimental information. The development, validation, and application of such a mechanistic model for the assessment of the transferability of the transpiration-use efficiency parameters across diverse climatic conditions was the main subject of this work.

In particular, the first chapter focuses on the development and description of a mechanistic canopy transpiration and photosynthesis model (CTP), which was used as standard to evaluate the transferability of the simple transpiration–based models of crop productivity. The main feature of the model is the partition of the canopy in sunlit and shaded fractions, a reliable alternative to model canopy fluxes based on concepts introduced by Sinclair et al. (1976), Fuchs et al. (1987), Petersen et al. (1992), and de Pury and Farquhar (1997). Model simulations were compared with transpiration estimated with weighing lysimeters for non stressed wheat and maize resulting in good agreement, although there was a slight tendency for the model to underestimate. The model calculates transpiration–use efficiency (w) as kg of CO_2 fixation per kg of water transpired. In order to express w as kg of aboveground biomass per kg of water transpired, a conversion factor (Monteith, 1981) of 0.33 was derived as a first approximation to compare simulated values of w with values obtained from literature. This factor was derived taking into account the fraction of gross photosynthesis lost by growth and maintenance respiration, the ratio of molecular weights of CH_2O and CO_2, and the portion of gross photosynthesis apportioned to the roots. Results showed that the average and standard deviation of the simulated w values were within the range of the observed data. The CTP model showed to be a suitable tool that required relatively easy–to–obtain input data and parameters, and that allowed a wide range of applications including different crops and weather conditions.

The second chapter of this dissertation was involved with the evaluation of the transferability of the parameters of simple transpiration–based models (k_{Da} and k_{ETo}) for wheat and maize across eight diverse climatic conditions. The CTP model was used for this purpose, with the advantage that the comparison of values of across climatic environments was made with a consistent methodology. The simulation results showed that w is not constant across climatic environments, so that values determined in one location can not be readily transferred to another. However, w as a function of D_a and ET_o was well described by a power function, with D_a explaining 94% and 90% of the w variability for wheat and maize, respectively, and ET_o explaining 89% and 72%, respectively. The dispersion around the fitted lines was lower with D_a and ET_o values greater than 2 kPa and 7 mm/day, respectively. Normalization by D_a and ET_o of the k_{Da} and k_{ETo} parameters was unable to properly account for the effect of weather variability, resulting in parameters that could not be readily transferred across locations for both wheat and maize. However, the transferability of these parameters was dramatically improved when they were plotted against D_a (in the case of k_{Da}) or ET_o (in the case of k_{ETo}), with linear functions describing well the relations and explaining 79% and 91% of k_{Da} variability for wheat and maize, and 71% of k_{ETo} variability for maize. The k_{ETo} for wheat correlated weakly with ET_o, explaining only 25% of its variability. However, the overall coefficient of variation of this parameter across eight locations was about 10%, so that the use of a constant k_{ETo} value is not unreasonable, although is not a perfect solution. The simulation–based equations developed in this chapter are offered as a first approximation to overcome the spatial transferability of w, k_{Da} and k_{ETo} .

In the third chapter the simulation–based equations from chapter 2 to estimate w, k_{Da} and k_{ETo} expressed in terms of CO_2 assimilation per unit ground area were converted to

aboveground biomass per unit ground area using a conversion factor f_{abg} (0.36 for wheat, and

0.33 for maize) optimized using observed field data. The variation of w with D_a was supported

by both observed and simulated data, with the simulation–based power equations showing to be

reliable estimators of w as function of D_a for wheat and maize. The simulation–based linear

equations to estimate k_{Da} as a function of D_a also showed to be good estimators of the observed

values for wheat and maize, with D_a able to explain most of the variation of k_{Da} across a wide

climatic range. Their use to extrapolate experimentally–determined k_{Da} values or to select k_{Da}

values for estimation of w and crop productivity is supported by these results. The performance

of functions to estimate k_{ETo} could not be tested with sufficient data, however some general

comments can be made: The use of an average k_{ETo} value appears a reasonable approximation to

estimate w of wheat while k_{ETo} for maize appeared correlated with variations of ET_o.

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Dedication

To my mentor professor Norbert Fritsch F.

To Coti, Catia and Catalina

Evaluating Simple Transpiration-based Models of Crop Productivity: Development of a

Reference Canopy Transpiration and Photosynthesis Model

ABSTRACT

There is a renewed interest in evaluating crop productivity using simple transpiration–based models of biomass accumulation. Transpiration–use efficiency (w), defined as the ratio of biomass (B) produced per unit water transpired (T), has been widely used to evaluate crop performance under limited water supply. Simple approaches to asses w have been used, including: 1) $w = k_{Da}/D_a$ and 2) $w = k_{ETo}/ET_o$; where k_{Da} and k_{ETo} are crop–dependent parameters, with the underlying concept that normalization by D_a or ET_o would account for the effects of climate variations on w, while k_{Da} or k_{ETo} would be reasonably constant across diverse environments. However, assessing the transferability of these parameters across locations is not easy because of the scarcity of experimentally–determined values for these parameters and the lack of consistency of the methodology used in the field experiments reported. For this reason, a canopy transpiration and photosynthesis model (CTP) was developed, tested, and applied to obtain simulated values of w, k_{Da} and k_{ETo} in different locations using a consistent methodology. Some features of the model include: (1) the partition of the canopy in sunlit and shaded fractions; (2) calculation of canopy solar radiation interception and averaged solar and PAR irradiance for sunlit and shaded leaves; (3) computation of canopy transpiration for each fraction using a big–leaf approach; (4) calculation of photosynthesis for an average sunlit and

shaded leaf and subsequent integration for the entire canopy; (5) leaf photosynthesis calculated by balancing the biochemical capacity for CO_2 fixation (demand) and the CO_2 flux from the surroundings (supply); (6) average leaf stomatal conductance (for sunlit and shaded canopy fractions), responsive to light, temperature, atmospheric CO_2 concentration, air vapor pressure deficit, and plant water status; (7) simulation of plant water uptake and the effect of plant water stress on leaf stomatal conductance. Model simulations were compared with evapotranspiration estimated with weighing lysimeters in non stressed wheat and maize. Statistical indices and graphical results showed good agreement between observed and simulated transpiration values for both crops, with the simulated values tracking well the daily fluctuations of the observed values. The model calculates transpiration–use efficiency (w) as kg of CO_2 assimilated per kg of water transpired. In order to express w as kg of aboveground biomass per kg of water transpired, as typically found in the literature, a conversion factor of 0.33 was used as a first approximation for both crops. The factor 0.33 accounts for the fraction of photosynthesis loss by respiration (growth and maintenance respiration), the ratio of molecular weights of CH_2O and CO_2, and the fraction of photosynthesis apportioned to the roots. Results showed that the average and standard deviation of the simulated w values were within the range of the observed data. Overall, the CTP model appears suitable to serve as reference to evaluate the transferability across climatic environments of simple models of biomass production based on transpiration–use efficiency.

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1. INTRODUCTION

An increasing need to evaluate crop productivity under limited or uncertain water supply scenarios has renewed interest in simple, transpiration–based models of crop productivity that can be readily applied to a large number of crop species across the range of climatic conditions where these crops are grown. Although these models were introduced as early as the beginning of the previous century, the experimental determination of the parameters (typically just one parameter) used in the models has been relatively scarce, probably due to the need of measuring crop transpiration for their determination. In addition, the experimental information has focused on a few crops and is largely insufficient for worldwide assessment of crop productivity.

As a result of scarce experimental information, it is not easy to assess the variability and transferability among locations of the parameters of these simple transpiration–based models. The problem is compounded because an important fraction of the variability can be traced back to the use in reported experiments of different crop varieties, crop management, methods of determination of transpiration rates, methods for biomass sampling, or to other sources of variability.

The development of a mechanistic model of canopy transpiration and photosynthesis (CPT model), which can be utilized as a tool to simulate the parameters of simple transpiration–based models, is a useful approach to evaluate the transferability of these parameters across diverse climatic conditions without the shortcomings of the available experimental information. The development of such a mechanistic model is the main subject of this chapter.

A major challenge to the development of the CTP model was to extract and adapt the advances in topics such as leaf photosynthesis (Farquhar et al., 1980), stomatal conductance

(Jarvis, 1976; Cowan, 1977, 1982; Ball et al., 1987) and the physics of transpiration (Monteith, 1963) from the scale of leaves to canopy. Canopy models can be categorized by their level of complexity in either big–leaf (e.g. Sellers et al., 1992; Dickinson et al., 1998) or multilayer models (e.g. Leuning et al., 1995; Wang and Jarvis, 1990). More recently, two–leaf models (sunlit and shaded leaf fractions) have re–emerged as a reliable alternative to model canopy fluxes. A few decades ago, Sinclair et al. (1976) discussed the advantages of using a two–leaf model to estimate photosynthesis by separately integrating (big–leaf assumption) the sunlit and shaded canopy fractions. This simplification is effective since photosynthesis in shaded leaves has a linear response to irradiance, whereas in sunlit leaves is independent of light because these are often light saturated, allowing to use the mean irradiance intercepted by each fraction, carrying a modest error in the prediction (de Pury and Farquhar, 1997). The approach was extended to transpiration, by integrating the parameters and variables that represent separately the bulk properties of sunlit and shaded canopy fractions (Fuchs et al., 1987; Petersen et al., 1992) with encouraging results. Compiling the earlier results, Wang and Leuning (1998) and Dai et al. (2004) developed two–leaf models for canopy photosynthesis and transpiration. These models were tested against field data (Leuning et al., 1998, Dai et al., 2004, respectively), indicating that model simulations were suitable and supporting the robustness of this approach.

Thus, the main objectives of this chapter were:

a) To develop a generic canopy transpiration and photosynthesis model (CTP), using a two–leaf approach, which can be used for diverse climatic conditions and for different agricultural crops.

b) To test model simulations of crop transpiration against field data for wheat and maize.

c) To test the model's ability to parameterize transpiration–use efficiency by comparison with field data for wheat and maize.

2. MODEL DESCRIPTION

A model to simulate canopy transpiration and photosynthesis (here after referred as CTP) was developed. The formulation of the model was based on abundant literature on canopy radiation, transpiration, and photosynthesis modeling, emphasizing the selection of methods and algorithms that utilize measurable inputs and that can be verified experimentally. The main features of the model are: (1) the partition of the canopy in sunlit and shaded fractions; (2) calculation of canopy solar radiation interception and average solar and PAR irradiance for sunlit and shaded leaves; (3) computation of canopy transpiration for sunlit and shaded fractions using a big–leaf approach; (4) calculation of photosynthesis for an average sunlit and shaded leaf and subsequent integration for the entire canopy; (5) leaf photosynthesis calculated by balancing the biochemical capacity for CO_2 fixation (demand) and the CO_2 flux from the surroundings (supply); (6) average leaf stomatal conductance (for sunlit and shaded canopy fractions), responsive to light, temperature, atmospheric CO_2 concentration, air vapor pressure deficit, and plant water status; (7) simulation of plant water uptake and the effect of plant water stress on leaf stomatal conductance. Inputs to the model are presented in Table (1). The model calculates dimensionless functions to estimate hourly climatic data from daily input data (see appendix A). Figures 1 and 2 show flow diagrams for the transpiration and photosynthesis submodels, applicable for both sunlit and shaded leaves.

Table1. List of the variables and parameters used by the model.

Inputs	Type	units
S_r	Daily global solar radiation	MJ m^{-2} day^{-1}
T_{max}	Daily maximum air temperature	^{o}C
T_{min}	Daily minimum air temperature	^{o}C
HR_{max}	Daily maximum relative humidity	-
HR_{min}	Daily minimum relative humidity	-
W	Average wind velocity	m s^{-1}
LAI	Green plant area index	-
LAI_{max}	Maximum LAI	-
h_{cmax}	Maximum crop height	m
z	Soil layer depth	m
d_z	Soil layer thickness	m
d_n	Number of soil layers	-
R_d	Root depth	m
ψ_e	Air entry water potential	J kg^{-1}
b	Campbell adjustment parameter	-
ψ_{fci}	Soil water potential at field capacity	J kg^{-1}
ψ_{lw}	Leaf water potential at the plant wilting point	J kg^{-1}
wc	Volumetric soil water content at field capacity	-
wp	Volumetric soil water content at wilting point	-
ρ_b	Soil layer bulk density	Mg m^{-3}
CO_2	Atmospheric CO_2 concentration	umol mol^{-1}
f_{abg}	Above ground biomass convertion factor	kg biomass kg^{-1} CO_2
K_c	Michaelis-Mentel constant for CO_2	umol mol^{-1}

K_o	Michaelis-Mentel constant for O_2	umol mol^{-1}
δ	Quantum efficiency for CO_2 uptake.	mol mol^{-1}
γ	Fraction of absorbed PAR radiation that is used for production of Rubisco.	
θ	Light-Rubisco colimitation factor	-
β	Sucrosa-Light-Rubisco colimitation factor (C_3)	-
β	CO_2-Light-Rubisco colimitation factor (C_4)	-
V_m	Maximum Rubisco capacity	umol m^{-2} s^{-1}
u	Initial slope of photosynthetic CO_2 response.	mol m^{-2} s^{-1}
$\delta\gamma$	Proportion of absorbed PAR related with the production of PEP carboxilase	-
g_{Dl}^{0}	Leaf stomatal conductance for CO_2 at 0 leaf to air vapor pressure deficit	mol m^{-2} s^{-1}
D_o	Empirical coefficient	kPa
fad	Adaxial fraction of total stomatal conductance.	-
fab	Abaxial fraction of total stomatal conductance.	-
g_s^{max}	Maximun leaf stomatal conductance for CO_2	mol m^{-2} s^{-1}
T_{leaf}	Optimal photosynthetic leaf temperature	^{0}C
x	Ratio of horizontal and vertical leaf elements of the mean projected canopy area for an ellipsoidal canopy.	-
L_w	Leaf width	m
$\Psi_{l,onset}$	Leaf water potential at the onset of water deficit-induced stomatal closure.	J kg^{-1}
$T_{p,onset}$	Full cover transpiration rate at the onset of stomatal closure.	mm hr^{-1}
$\Psi_{1/2}$	Empirical coefficient representing the value of the leaf water potential when stomatal conductance is a half maximum.	J kg^{-1}
n	Fitted coefficient for leaf water potential calculation	-
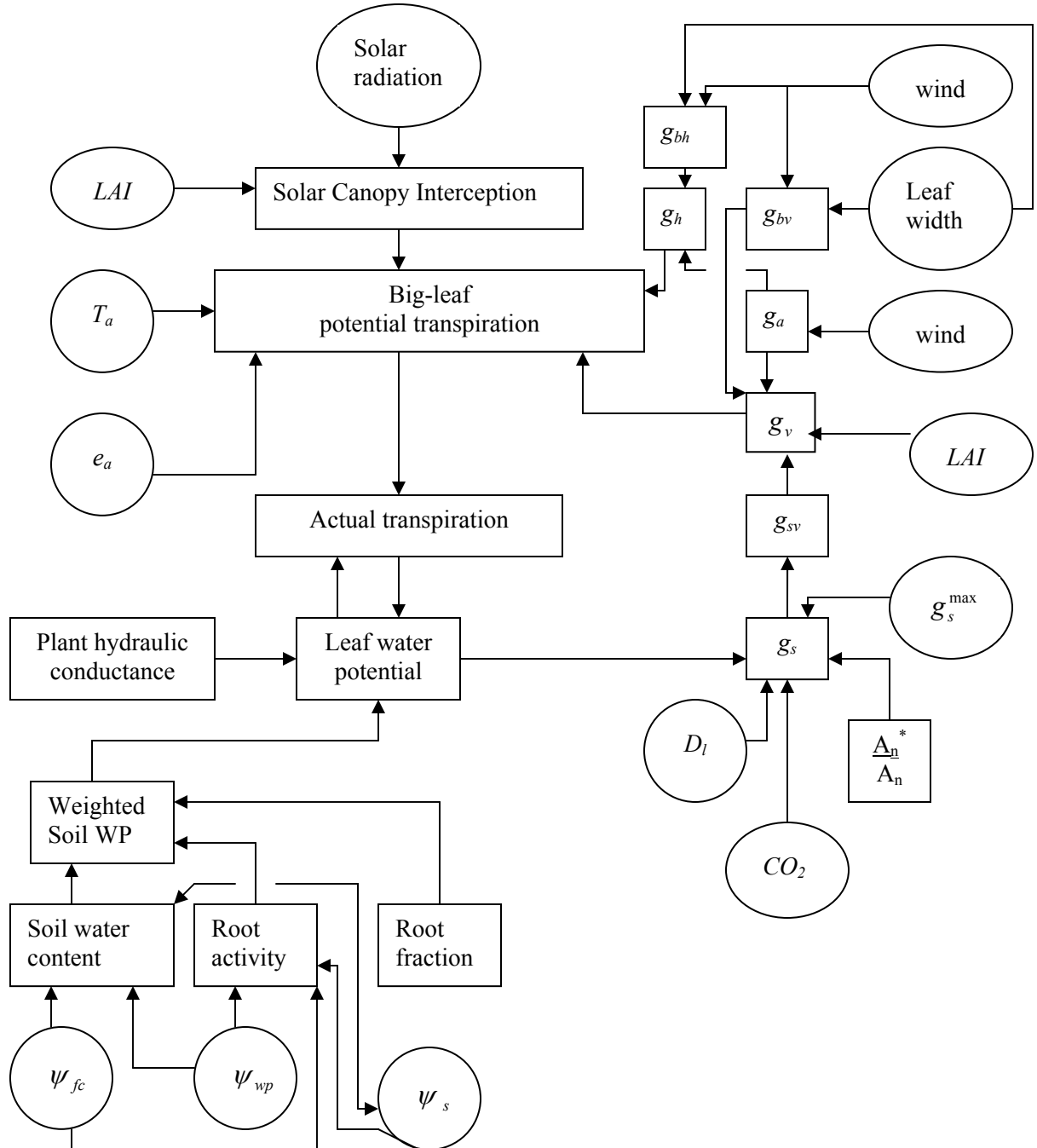
Figure 1. Model diagram for sunlit or shaded leaves transpiration. Where A_n* and A_n are reference and current photosynthesis for an average leaf, T_a and T_l are air and leaf temperature, e_a is the air vapor pressure, D_l is the leaf to air vapor pressure deficit , LAI is the green leaf area index, g_s and g_{sv} are the average leaf stomatal conductance for CO_2 and water vapor, g_a is the aerodynamic conductance, g_h and g_v are the canopy heat and water vapor conductance, g_{bv} and g_{bh} are boundary layer conductance for water vapor and heat, ψ_s is the soil water potential, ψ_{fc}, ψ_{wp} are the soil water potential at field capacity and at wilting point and g_s^{max} is the maximum stomatal conductance to CO_2.

Figure 2. Model diagram for sunlit or shaded leaves photosynthesis. Where A_n* and A_n are the reference and current photosynthesis for an average leaf, D_l is the leaf to air vapor pressure deficit, CO_2 is referred as the atmospheric CO_2 concentration, g_s^{max} is the maximum stomatal conductance to CO_2, g_{bh} and g_{bc} are the heat and CO_2 boundary layer conductance, g_s is stomatal conductance to CO_2 , g_a is the aerodynamic conductance LAI is the green leaf area index, f_{abg} is a conversion factor and $\lambda_v E_l$ is the expected leaf latent heat.

2.1. Canopy Radiation

2.1.1. Direct and diffuse short wave irradiance

Following a set of functions proposed by Liu and Jordan (1960), the model partitions the global solar irradiance into beam irradiance (S_b; J s^{-1}m^{-2}) and diffuse irradiance (S_d; J s^{-1}m^{-2}) as:

$$S_d = 0.3(1 - \tau^m)S_p \tag{1}$$

where m is the optical air mass number, S_p is the extraterrestrial flux density irradiance (J s^{-1}m^{-2}) at a horizontal surface outside the earth's atmosphere, and τ is the atmospheric transmittance.

The optical air mass number is obtained as:

$$m = \frac{P_a}{101.3\cos\lambda} \tag{2}$$

where P_a is the atmospheric pressure (kPa), and λ is the zenith angle (angle of the sun measured from the vertical) in radians.

The hourly extraterrestrial flux density irradiance (S_p, J s^{-1}m^{-2}) is determined as:

$$S_p = 1360d^2\cos\lambda \tag{3}$$

where the number 1360 (J s^{-1}m^{-2}) is the solar constant (Weiss and Norman, 1985), and the term d^2 adjusts for variation in earth-sun distance over the year which is obtained as:

$$d^2 = 1 + 0.0334\cos(0.01721\,DOY - 0.0552) \tag{4}$$

In addition:

$$\lambda = \arccos(\sin\phi\sin\delta + \cos\phi\cos\delta\cos 0.2618(h-12)) \tag{5}$$

$$\sin\delta = 0.39785\sin(4.869 + 0.0172DOY + 0.03345\sin(6.224 + 0.0172DOY)) \tag{6}$$

where ϕ is the latitude expressed in radians, δ is solar declination in radians, DOY is the day of the year and h is the standard local time in hours.

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Values of τ determined in clear sky conditions have been reported by Gates (1980) ranging from 0.45 to 0.75. This model defines τ as:

$$\tau = \frac{S_r}{S_p}; \qquad \text{if} \quad \tau > 0.75 \Rightarrow \tau = 0.75$$

$$\text{if} \quad \tau < 0.45 \Rightarrow \tau = 0.45 \qquad (7)$$

where S_r/S_p is the ratio of hourly solar irradiance to hourly extraterrestrial solar irradiance.

Hourly solar irradiance (J s^{-1}m^{-2}) is determined as:

$$S_r = S_{rd} \frac{S_p}{S_{pd}} \qquad (8)$$

where S_{rd} is the observed daily solar irradiance and S_p/S_{pd} is the hourly fraction of the daily extraterrestrial solar irradiance. The daily extraterrestrial flux density irradiance (S_{pd}, J s^{-1}m^{-2}) is obtained as:

$$S_{pd} = \int_0^{24} S_p dh \qquad (9)$$

Finally, the beam irradiance (S_b; J s^{-1}m^{-2}) is obtained as:

$$S_b = S_r - S_d \qquad (10)$$

2.1.2. Transmission of beam irradiance

The fraction of incident beam irradiance (τ_{bt}) that penetrates the canopy and reaches the soil surface at a given solar zenith angle (λ) is a function of the green leaf area index (*LAI*), and is assessed by:

$$\tau_{bt}(\lambda) = \exp(-\alpha^{0.5} K_b(\lambda) LAI) \qquad (11)$$

where the term α corresponds to leaf absorptivity, and $\alpha^{0.5}$ intends to account for scattering due to transmission and reflection by the leaves (Goudriaan, 1977). The extinction coefficient $K_b(\lambda)$ is the fraction of *LAI* which creates a plane projected shadow over a horizontal surface from a particular zenith angle. The extinction coefficient is modeled assuming an ellipsoidal leaf angle distribution (Campbell and Norman, 1998):

$$K_b(\lambda) = \frac{\left(x^2 + \tan^2(\lambda)\right)^{0.5}}{\left(x + 1.774(x + 1.182)^{-0.733}\right)} \tag{12}$$

where x is the ratio of horizontal and vertical leaf elements of the mean projected canopy area. This value is selected to represent canopies with vertical, horizontal or spherical leaf angle distribution.

2.1.3. Transmission of diffuse irradiance

Diffuse unlike beam irradiance comes from all directions, so that its transmission through the canopy can be obtained by integration of τ_{bt} and can be estimated using the following equation (Ross, 1975):

$$\tau_d = 2 \int_0^{\pi/2} \tau_{bt}(\lambda) \sin\lambda \cos\lambda \, d\lambda \tag{13}$$

2.1.4. Global irradiance reflected by the canopy

The reflection of global irradiance by a dense canopy is computed as proposed by Goudriaan (1988):

$$\rho_{cpy}(\lambda) = \frac{2K_b(\lambda)}{K_b(\lambda) + K_d^b} \rho_{cpy}^{HZ} \tag{14}$$

where $\rho_{cpy}(\lambda)$ is the reflection coefficient (albedo) of the canopy as a function of the zenith angle and, K_d^b is the diffusive extinction coefficient for black leaves computed as:

$$K_d^b = -Ln\frac{\tau_d}{LAI} \tag{15}$$

where τ_d is assessed with equation 13, considering $\alpha = 1$ (black leaves) and, ρ_{cpy}^{HZ} is the canopy hemispherical reflection coefficient for leaves horizontally oriented given by:

$$\rho_{cpy}^{HZ} = \frac{1-\sqrt{\alpha}}{1+\sqrt{\alpha}} \tag{16}$$

2.1.5. Absorption of global solar radiation by the canopy

The model assumes that S_b is intercepted by the sunlit fraction of the canopy, and S_d is partitioned over the sunlit (LAI_{su}) and shaded (LAI_{sh}) leaf area of the canopy hence:

$$S_{su} = \left[S_b(1-\tau_{bt}(\lambda))+\frac{LAI_{su}}{LAI}S_d(1-\tau_d)\right](1-\rho_{cpy}(\lambda)) \tag{17}$$

$$S_{sh} = \frac{LAI_{sh}}{LAI}S_d(1-\tau_d)(1-\rho_{cpy}(\lambda)) \tag{18}$$

where S_{su} and S_{sh} are the solar radiation absorption by the sunlit and shaded leaves (J s^{-1}m^{-2}), respectively. The sunlit leaf area index is determined as (Campbell and Norman, 1998):

$$L_{su} = \frac{1-\exp[K_b(\lambda)LAI]}{K_b(\lambda)} \tag{19}$$

Thus the shaded leaf area index is given by:

$$LAI_{sh} = LAI - LAI_{su} \tag{20}$$

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2.1.6. Global and PAR solar irradiance within the canopy

2.1.6.1. Global Solar Irradiance

The average solar irradiance on sunlit leaves is obtained as:

$$S_{su}^{av} = K_b S_b + S_{sh}^{av} \tag{21}$$

where S_{sh}^{av} is the average solar irradiance (J s^{-1}m^{-2}) on shaded leaves compose by the canopy average diffuse $\left(S_d^{av}\right)$ plus scattered $\left(S_{sc}^{av}\right)$ solar irradiance. The fraction of diffuse solar irradiance transmitted down the canopy is assessed by:

$$S_d^{av} = S_d \exp\left(-\alpha^{0.5} K_d LAI\right) \tag{22}$$

and the down–scattered solar irradiance is given by:

$$S_{sc}^{av} = S_{gl} - S_{bl} \tag{23}$$

where S_{gl} is the unintercepted beam plus down scattered solar beam irradiance and S_{bl} is unintercepted solar beam irradiance , determined as:

$$S_{gl} = S_b \exp(-\alpha^{0.5} K_b LAI) \tag{24}$$

$$S_{bl} = S_b \exp(-K_b LAI) \tag{25}$$

The model estimates a canopy average value of $S_d^{av} + S_{sc}^{av}$. The canopy LAI is split into multiple layers (increments in LAI of 0.1 from the top). At the end, every layer value of $S_d^{av} + S_{sc}^{av}$ is added and averaged by the number of layers.

2.1.6.2. Photosynthetically Active Irradiance (PAR)

The mean PAR flux density (J s^{-1}m^{-2}) on sunlit leaves (R_{su}) is given by (Campbell and Norman 1998):

$$R_{su} = K_b R_b + R_{sh} \tag{26}$$

where R_b is the beam PAR flux density at the top of the canopy given by:

$$R_b = 0.5 S_b \tag{27}$$

and R_{sh} is the mean PAR flux density (J s^{-1}m^{-2}) on shaded leaves compose by the canopy average diffuse (R_d) plus scattered (R_{sc}) PAR. The fraction of diffuse PAR transmitted down the canopy is assessed by:

$$R_d = 0.5 S_d \exp\left(-\alpha^{0.5} K_d LAI\right) \tag{28}$$

and the down-scattered PAR is given by:

$$R_{sc} = R_{gl} - R_{bl} \tag{29}$$

where R_{gl} is the unintercepted beam plus down scattered beam PAR and R_{bl} is unintercepted beam PAR, determined as:

$$R_{gl} = R_b \exp(-\alpha^{0.5} K_b LAI) \tag{30}$$

$$R_{bl} = R_b \exp(-K_b LAI) \tag{31}$$

The procedure to finally asses R_{sh} as a canopy average of $R_d^v + R_{sc}$ from equation 28 through 31 is the same already explained to obtain S_{sh}^{av}.

2.2. Canopy Transpiration

Canopy transpiration is estimated as the sum of transpiration from the sunlit and shaded fractions of the canopy. For each fraction transpiration is calculated solving the canopy (big–leaf) energy balance to obtain latent heat loss ($\lambda_v E_c$ in J m^{-2} s^{-1}). Transpiration is then given by the quotient between latent heat loss and the latent heat of vaporization ($\lambda_v \approx 44000$ J mol^{-1}).

2.2.1. Canopy energy balance

The canopy energy balance assuming that heat storage and metabolic heat production are negligible is given by:

$$S_{abs} - L_c - H - \lambda_v E_c = 0 \tag{32}$$

where S_{abs} is the radiation absorbed by the canopy (J s^{-1}m^{-2}), L_c is the emitted long wave radiation (J s^{-1}m^{-2}), H is the sensible heat (J s^{-1}m^{-2}), and $\lambda_v E_c$ is the canopy latent heat loss (J s^{-1}m^{-2}). The radiation absorbed by the canopy is obtained as:

$$S_{abs} = S + L_a \tag{33}$$

where S is the solar radiation absorption (J s^{-1}m^{-2}, either S_{su} or S_{sh}), and L_a is the emitted long wave radiation from the sky (J s^{-1}m^{-2}) computed as:

$$L_a = \varepsilon_s \sigma T_a^{\,4} \tag{34}$$

where ε_s is the sky longwave emissivity, σ is the Stephan Boltzmann constant (5.67 x 10^{-8} J s^{-1} m^{-2} K^{-4}), and T_a is the air temperature (°K). The sky longwave emissivity is given by:

$$\varepsilon_s = (1 - 0.84 f_c)\varepsilon_{sc} + 0.84 f_c \tag{35}$$

and
$$\varepsilon_{sc} = 1.72\left(\frac{e_a}{T_a}\right)^{1/7} \tag{36}$$

$$f_c = 1.35\left(\frac{S_r}{0.75 S_p}\right) - 0.35 \tag{37}$$

where f_c is a cloudiness factor, ε_{sc} is the clear sky longwave emissivity and, e_a is the air vapor pressure (kPa). The long wave radiation emitted by the canopy (L_c) is obtained as:

$$L_c = \varepsilon_c \sigma T_c^{\,4} \tag{38}$$

where ε_c is the canopy emissivity $(\varepsilon_c = 0.97)$ and T_c is the mean canopy temperature (°K). The sensible heat (H) is estimated as:

$$H = c_p g_h (T_a - T_c)$$ (39)

where c_p is the air specific heat ($c_p = 29.3$ J mol^{-1} °C^{-1}), T_a and T_c are the air and canopy temperatures (°C) and g_h is the canopy heat conductance (mol m^{-2} s^{-1}).

Canopy latent heat $(\lambda_v E_c)$ assessment is given by:

$$\lambda_v E_c = \lambda_v g_v \left(\frac{e_c - e_a}{P_a} \right)$$ (40)

where λ_v is the latent heat of vaporization ($\lambda_v \approx 44000$ J mol^{-1}), e_c is the mean canopy vapor pressure (kPa), e_a is the air vapor pressure, P_a is the atmospheric pressure (kPa) and, g_v is the canopy conductance to water vapor (mol m^{-2} s^{-1}).

2.2.2. Conductances for water vapor and heat exchange

Conductances values for vapor and heat exchange must be determined. In both cases a common aerodynamic conductance is calculated based on crop height and wind speed (Campbell and Norman, 1998) as:

$$g_a = \frac{0.4^2 \rho_a u_e}{\left[\ln\left(\frac{z - d + z_M}{z_M} \right) \right]\left[\ln\left(\frac{z - d + z_H}{z_H} \right) \right]}$$ (41)

where u_e is the wind velocity (m s^{-1}) at 1 m above the canopy height (h_c in m), d is the zero plane displacement (m) taken as $0.65 h_c$, z_M and z_H are the momentum and sensible heat roughness parameters (m), 0.4 is the von Karman's constant and, ρ_a is the air molar density (J mol^{-1} K^{-1}). Roughness parameters were estimated using the following:

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$$z_M = 0.1h_c \tag{42}$$

$$z_H = 0.2z_M \tag{43}$$

2.2.2.1. Total conductance to water vapor exchange

The water vapor conductance for either the sunlit or shaded fraction of the canopy (g_v) is the resultant of three partial conductances added in series; aerodynamic conductance (g_a), stomatal conductance to water vapor (g_{sv}), and the boundary layer conductance to water vapor (g_{bv}) as :

$$g_v = \frac{1}{\dfrac{1}{\left(\dfrac{g_{sv}g_{bv}}{g_{sv}+g_{bv}}\right)LAI} + \dfrac{1}{g_a}} \tag{44}$$

where the product $\left(\dfrac{g_{sv}g_{bv}}{g_{sv}+g_{bv}}\right)LAI$ is the leaf water vapor conductance of a typical leaf integrated over the canopy green leaf area index (sunlit or shaded).

The stomatal conductance to water vapor is given by:

$$g_{sv} = 1.56\, g_s \tag{45}$$

where g_s is the stomatal conductance to CO_2, its assessment is explained later in section (2.3.2.1.), and 1.56 accounts for the differences in molecular diffusion rate of water vapor and CO_2.

The boundary layer conductance for water vapor is estimated as :

$$g_{bv} = 1.4 x 0.147\sqrt{\dfrac{u}{d_l}} \tag{46}$$

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where u is the wind speed (m s^{-1}) at the top of the canopy (u_t) for sunlit leaves, within the

canopy (u_c) for shaded leaves, and d_l is the leaf characteristic length (m).

2.2.2.2. Total heat conductance

The canopy heat conductance for either the sunlit or shaded fraction of the canopy (g_h)

is assessed as:

$$g_h = \frac{1}{\dfrac{1}{g_a} + \dfrac{1}{(g_{bh}LAI)}} \tag{47}$$

where the product $(g_{bh} LAI)$ is the heat boundary layer conductance of a typical leaf integrated

over the canopy green leaf area index (sunlit or shaded) and g_{bh} is the boundary layer

conductance for heat estimated as:

$$g_{bh} = 1.4x0.135\sqrt{\frac{u}{d_l}} \tag{48}$$

where u is the wind speed (m s^{-1}) at the top of the canopy (u_t) for sunlit leaves, and within the

canopy (u_c) for shaded leaves, and d_l is the leaf characteristic length (m).

2.2.3. Wind velocity for aerodynamic and boundary layer calculations

Wind velocity (m s^{-1}) is computed from field data to four different heights, 10 m above

the soil surface, 1 m above the top of the canopy, at the top canopy, and within the canopy. An

equation which account for the wind velocity at a height z (m) above the soil surface is given by

(Thom, 1975; Campbell and Norman, 1998):

$$u_z = \frac{u^*}{0.4} \ln \frac{z-d}{z_M} \tag{49}$$

where u_z is the wind velocity at a height z above soil surface, u^* is the friction velocity (m s^{-1}),

and z_M is the momentum roughness parameters (m). Equation 42 describes the method to

compute z_M. Using Eq. (49) and the daily data of wind velocity (assuming that for a standard

weather station wind sensors are above a surface of green grass of uniform height of 0.12 m) the

model computes a reference friction velocity by solving for u^*, and then calculates wind

velocity at a reference plane located 10 m above the soil surface using again Eq. (49) with the

calculated u^*. Once the velocity at the reference plane is computed, the wind velocity at the top

of the canopy (u_t) and at a plane 1 m above the canopy top (u_e) is assessed using Eq. (49) with

$z = h_c$ and $z = h_c + 1$, respectively, where h_c is the crop height.

The wind velocity within the canopy (u_c, m s^{-1}) is given by (Thom, 1975; Petersen et al.,

1992) :

$$u_c = u_t \exp(-\xi \upsilon) \tag{50}$$

where ξ is an attenuation factor given by:

$$\xi = 1.5 + \frac{LAI}{3} \tag{51}$$

and υ is the fractional leaf area index:

$$\upsilon = 1 - \frac{LAI_{sh}}{LAI} \tag{52}$$

2.3. Canopy Photosynthesis

Leaf photosynthesis is computed balancing the biochemical capacity for CO_2 fixation (demand) and the CO_2 flux from the surroundings to the intercellular spaces within the leaf (supply). Canopy photosynthesis is estimated by integration over the leaf area of the photosynthesis of an average sunlit and shaded leaf.

2.3.1. CO_2 demand

The model of leaf photosynthesis presented by Collatz et al. (1991) (C_3 assimilation pathway), and Collatz et al. (1992) (C_4 assimilation pathway), were adopted for the calculation of net assimilation (A_n). Net assimilation is computed as the minimum of three potential CO_2 uptake rate capacities: light–limited rate (J_E), Rubisco–limited rate (J_R), and either the rate imposed by sucrose synthesis (J_S, C_3 plants) or the CO_2–limited rate (J_C, C_4 plants) as:

$$A_n = \min\{J_E, J_C, J_S \text{ or } J_C\} - R_d \tag{53}$$

where R_d symbolizes the cost of the leaf photosynthesis as 'day' respiration rate.

2.3.1.1. C_3 assimilation pathway

The light limited assimilation rate (J_E, umol m^{-2} s^{-1}) is given by:

$$J_E = \frac{\alpha \, \delta \, R \left(C_i - \Gamma^*\right)}{C_i + 2\Gamma^*} \tag{54}$$

where α is the absorptivity of the leaf for PAR, δ is the intrinsic quantum efficiency for CO_2 uptake (mol mol^{-1}, maximum number of CO_2 molecules fixed per quantum of radiation absorbed), R is the PAR flux density irradiance on the leaf in (umol m^{-2}s^{-1}), C_i is the intercellular CO_2 concentration (umol mol^{-1}), and Γ^* is the light compensation point, which is calculated as:

$$\Gamma^* = \frac{C_o}{2\omega} \tag{55}$$

where C_o is the oxygen concentration in air ($C_o = 210$ mmol mol^{-1}), and ω is a ratio describing the portioning of the carboxylase and oxigenase reactions of Rubisco ($\omega = 2.6$ mmolumol^{-1}). The Rubisco–limited assimilation rate (J_c, umol m^{-2} s^{-1}) is computed as:

$$J_R = \frac{V_m\left(C_i - \Gamma^*\right)}{C_i + K_c\left(1 + \dfrac{C_o}{K_o}\right)} \tag{56}$$

where V_m is the maximum Rubisco capacity per unit area (umol m^{-2} s^{-1}), K_o (mmol mol^{-1}) and K_c (umol mol^{-1}) are the Michaelis–Menten constants for O_2 and CO_2. When the concentration of photosynthesis products raises and the use and export of these products are limited, a slower reaction is imposed. This effect is accounted through the sucrose synthesis (Js, umol m^{-2} s^{-1}) rate given by:

$$J_S = \frac{V_m}{2} \tag{57}$$

Equations 54, 56 and 57 imply a sharp transition from one rate limiting process to another. In reality there is a more gradual transition, with some co–limitation when two rates are nearly equal. This gradual transition is modeled empirically using quadratic functions as follows:

$$J_p = \frac{J_E + J_R - \sqrt{\left(J_E + J_R\right)^2 - 4\theta J_E J_R}}{2\theta} \tag{58}$$

and

$$A = \frac{J_p + J_S - \sqrt{\left(J_p + J_S\right)^2 - 4\beta J_p J_S}}{2\beta} \tag{59}$$

where J_p is a intermediate variable representing the minimum of J_E and J_C. Photosynthesis (A_n, umol m^{-2}s^{-1}) is assessed as a result of the second limitation imposed by computing the minimum

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of J_p with J_S. The terms θ and β are empirical constants which control the sharpness of the transition between limitations.

The rate of respiration (Rd; umolm^{-2}s^{-1}) is computed as:

$$R_d = 0.015Vm \tag{60}$$

Temperature effects on photosynthesis are accounted by effects on some of the model parameters. The parameters K_c, ω and K_o are adjusted by temperature as follows:

$$k = k_{25} \exp\left[q\left(T_l - 25\right)\right] \tag{61}$$

where k is the modified parameter, k_{25} is the value of the parameters at 25 degrees Celsius, q is the temperature coefficient for the correspond parameter, and T_l is the mean leaf temperature (°C). The q coefficients for K_c, ω, and K_o are 0.074, -0.056, and 0.018, respectively. The parameter V_m is also corrected by temperature using the following function:

$$V_m = \frac{V_{m25} \exp\left[0.088\left(T_l - 25\right)\right]}{1 + \exp\left[0.29\left(T_l - 41\right)\right]} \tag{62}$$

and

$$R_d = \frac{R_{d25} \exp\left[0.069\left(T_l - 25\right)\right]}{1 + \exp\left[1.3\left(T_l - 55\right)\right]} \tag{63}$$

2.3.1.2. C$_4$ assimilation pathway

Collatz et al. (1992) proposed a simplified model to estimated leaf net photosynthesis for C$_4$ metabolism. These authors hypothesized that the light–limited rate of photosynthesis, under conditions where the partial pressure of CO_2 in the bundle sheath chloroplast is sufficiently high to suppress photorespiration is given by:

$$J_E = \alpha \; \delta \gamma R \tag{64}$$

where α is the absorptivity of the leaf for PAR, δ is the intrinsic quantum efficiency for CO_2 uptake (mol mol^{-1}), R is the PAR flux density irradiance on the leaf in (umol m^{-2}s^{-1}) and, γ is the fraction of absorved R that is used for production of Rubisco. The model combines the product of $\delta\gamma$ in a single constant with a theoretical value of 0.067 (mol mol^{-1}).

The CO_2 limited rate $\left(J_C\right)$ is given by:

$$J_C = \mu\, C_i \tag{65}$$

where μ is the slope of the CO_2 (mol m^{-2} s^{-1}) responses curve at low internal CO_2.

When the rate of assimilation is not limited by light and CO_2, the rate is instead defined by the capacity to attach CO_2 by Rubisco. Under these conditions, the concentration of CO_2 on the bundle sheath chloroplast nearly saturates Rubisco activity, and then:

$$J_R = V_m \tag{66}$$

Respiration (Rd) and finally net photosynthesis (A_n) are computed using the same route than $C3$ plants.

The co–limitation of J_E, J_R, and J_C is determined as explained before for C_3 assimilation pathway, where J_S in equation 57 is replaced by J_C.

Temperature adjustments of V_m and μ are performed as follows:

$$V_m = 1.065215 \frac{V_{m25}\, Q_{10}^{\frac{T_l-25}{10}}}{\left(1+\exp 0.3\left(13-0.3T_l\right)\right)\left(1+\exp 0.3\left(T_l-36\right)\right)} \tag{67}$$

$$u = u_{25}\, Q_{10}^{\frac{T_l-25}{10}} \tag{68}$$

where V_{m25} and μ_{25} are the parameter's values at 25 degrees Celsius, and Q_{10} is the proportional increase in a parameter value for a 10 $^{\circ}$C increase in leaf temperature.

2.3.1.3. Mean temperature for sunlit and shaded leaves

Leaf temperature is computed by solving the energy balance equation for an average sunlit or shaded unit leaf area as:

$$\alpha S^{av} + \varepsilon_s \sigma T_{wc}^{\ 4} - \varepsilon_c \sigma T_l^{\ 4} - c_p g_{bh}(T_{wc} - T_l) - \lambda_v E_l = 0 \tag{69}$$

where α is the leaf absortivity (0.5), S^{av} is the average sunlit $\left(S_{su}^{av}\right)$ or shaded $\left(S_{sh}^{av}\right)$ leaf solar irradiance (J s^{-1}m^{-2}, see their computation in 2.1.6.1. Global Solar Irradiance), T_l and T_{wc} are the leaf and within the canopy air temperature (^{o}K or ^{o}C; see differences of use in canopy energy balance section), g_{bh} is the leaf heat boundary layer (mol m^{-2} s^{-1}), $c_p, \sigma, \varepsilon_s$ and ε_c have the same meaning already explained in the canopy energy balance, and $\lambda_v E_l$ is the expected leaf latent heat (J s^{-1}m^{-2}). The latter is given by the canopy latent heat loss calculated using a big–leaf approach scaled to a unit leaf area.

The temperature within the canopy is given by:

$$T_{wc} = T_a + \frac{H_{su} + H_{sh}}{c_p g_a} \tag{70}$$

where H_{su} and H_{sh} are the sensible heat fluxes (J s^{-1}m^{-2}) for the canopy sunlit and canopy shaded fraction and g_a is the aerodynamic conductance.

The expected leaf latent heat flux per unit leaf area is determined by the canopy latent heat loss expressed per unit leaf area as:

$$\lambda_v E_l = \frac{\lambda_v E_c}{LAI} \tag{71}$$

where $\lambda_v E_c$ and LAI are either for sunlit or shaded leaves.

2.3.2. CO_2 Supply

The CO_2 gas exchange between the atmosphere and the intercellular spaces of the leaf is described by Fick's law as:

$$A_n = g_{tc}(C_a - C_i)$$ (72)

where g_{tc} is the leaf conductance for CO_2 (mol m^{-2}s^{-1}), C_a is the atmospheric CO_2 concentration (umol mol^{-1}) and C_i is the leaf intercellular CO_2 concentration (umol mol^{-1}). The value of C_i is obtained through iteration until equilibrium between CO_2 demand and supply is reached. Once the C_i for equilibrium is determined, leaf net assimilation is given by:

$$A_n = g_{tc}C_a\left(1 - \frac{C_i}{C_a}\right)$$ (73)

2.3.2.1. Total conductance for CO_2 transfer

The CO_2 total leaf conductance for (g_{tc}, mol m^{-2}s^{-1}) is the expression of three partial conductances on series: aerodynamic conductance (g_a, mol m^{-2} s^{-1}), boundary layer conductance of CO_2 (g_{bc}, mol m^{-2}s^{-1}), and stomatal conductance of CO_2 (g_s, mol m^{-2}s^{-1}) as:

$$g_{tc} = \frac{1}{\dfrac{1}{\dfrac{g_s g_{bc}}{g_s + g_{bc}}} + \dfrac{1}{g_a}}$$ (74)

The aerodynamic conductance is computed as mentioned in section 2.2.2. The CO_2 boundary layer conductance is computed after Campbell and Norman (1998) as follows:

$$g_{bc} = 1.4 x 0.11\sqrt{\frac{u}{d_l}}$$ (75)

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where u is the wind speed at the top of the canopy (u_t) for an average sunlit leaf and inside the canopy (u_c) for an average shaded leaf, and d_l is the leaf characteristic length.

The correct parameterization of CO_2 stomatal conductance (g_s) is essential in the simulation of crop productivity, affecting both photosynthesis and transpiration (Yu et al., 2004). Jarvis (1976) developed an empirical model to predict stomatal conductance using the maximum stomatal conductance (g_s^{max}) for the plant species multiplied by non interactive correction coefficients representing the independent effect of solar irradiance (S), leaf temperature (T_l), air vapor pressure deficit (D_a), atmospheric CO_2 concentration (C_a), and leaf water status (ψ_l) as:

$$g_s = g_s^{max} f_s \, f_{Tl} \, f_{Da} f_{Ca} \, f_{\psi l} \tag{76}$$

Another semi–empirical model was presented by Ball et al. (1987), based on previous concepts by Wong et al. (1979), and Wong et al. (1985 a, b, c), that partitioned the responses of stomata to changes in the environment into components that are dependent on photosynthesis and others that are independent of photosynthesis as:

$$g_s = b + m \frac{A_n h_s}{C_s} \tag{77}$$

where A_n is the leaf net photosynthesis rate, h_s is relative humidity and C_s is the CO_2 concentration of air at the leaf surface. The parameters m and b are the slope and intercept of the equation respectively and must be determined empirically.

Equation 77 can be redefined by replacing the effects of the relative humidity with a hyperbolic function of humidity deficit (f_{Dl}, Leuning, 1995), introducing a water stress function (f_w, see development of this factor later), and assuming that b is negligible for active plants under no severe water stress yielding the following form:

$$g_s = m \frac{A}{C_s} f_{Dl} f_w \tag{78}$$

With f_{Dl} defined as

$$f_{Dl} = \frac{g_{Dl}^0}{g_s^{max}\left(1 + D_l/D_o\right)}; \text{ if } f_{Dl} > 1 \text{ then } f_{Dl}=1 \tag{79}$$

where D_l is the leaf to air vapor pressure difference, and g_{Dl}^0 and D_o are fitted parameters of a hyperbolic function of humidity deficit to estimate g_s

For a given atmospheric CO_2 concentration, a maximum value of g_s $\left(g_s^{max}\right)$ can be observed for the following condition: no water stress $\left(f_w \approx 1\right)$, photosynthesis operating at optimum light and temperature (A_n^*), and high air humidity $\left(f_{Dl} \approx 1\right)$. Under this condition Eq. (78) can be written as:

$$g_s^{max} = m \frac{A_n^*}{C_s} \tag{80}$$

Assuming proportionality between g_s and A_n^*, a relative stomatal conductance, expressed as fraction g_s^{max} is given by:

$$\frac{g_s}{g_s^{max}} = \frac{A_n}{A_n^*} f_{Dl} f_w \tag{81}$$

Rearranging equation 81 a hybrid stomatal conductance model which has physiological relationships similar to the Ball et al. (1987) model but introduce the effects of plant water stress and humidity like the Jarvis type model is obtained:

$$g_s = g_s^{max} f_{Dl} f_w \frac{A_n}{A_n^*} \tag{82}$$

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Equation 82 requires g_s^{max}, which is well documented for many crops (eg : Körner et al.,

1979; Körner , 1994; Kelliher et al., 1995; Monteith, 1995). However, g_s^{max} is also dependent

of atmospheric CO_2 concentration. Therefore, a CO_2 adjustment factor (f_{CO2}) must be

introduced to Eq. (82):

$$g_s = g_s^{max} f_{CO2} f_{Dl} f_w \frac{A_n}{A_n^*}$$ (83)

The CO_2 adjustment factor is given by:

$$f_{CO2} = 1 - \frac{\left(C_a - C_a^{ref}\right)S_{CO2}}{g_s^{max}}$$ (84)

where C_a^{ref} is the reference atmospheric CO_2 (atmospheric CO_2 concentration at the time when

g_s^{max} was recorded), and S_{CO2} is a sensitivity constant (0.001212 mol m^{-2} s^{-1} stomatal

conductance change per umol mol^{-1} change in atmospheric CO_2 concentration), adapted from

Morison (1987).

The water stress function (f_w) depends on the soil water budget (see development of this

later) and describes relative stomatal conductance as a function of leaf water potential (Fischer et

al., 1981; Jones, 1992):

$$f_w = \frac{1}{\left(1 + \bar{\psi_l}/\psi_{1/2}\right)^n}$$ (85)

where $\bar{\psi_l}$ is the mean leaf water potential (J kg^{-1}) either for sunlit or shaded leaves, $\psi_{1/2}$ is the

value of $\bar{\psi_l}$ (J kg^{-1}) when g_s is half maximum and n is a fitted coefficient.

2.4. Crop Water Stress

Crop water stress, and its effect on stomatal conductance through Eq. (85), depends on actual crop transpiration compared to the potential crop transpiration with no stress. The mean leaf water potential, the crop water status, and the actual transpiration rate are determined by the equilibrium between liquid water uptake from the root zone and water vapor loss as transpiration. The modeling approach used was based on the principles proposed by Campbell (1985) and the work by Stöckle and Jara (1998). The water potential is highest in the soil and decreases along the transpiration path. This potential gradient provides the driving forces to liquid water transport from the soil to the sites of evaporation in the canopy leaves. Figure 3 shows an electric analog of the water path showing the most important conductances and potentials.
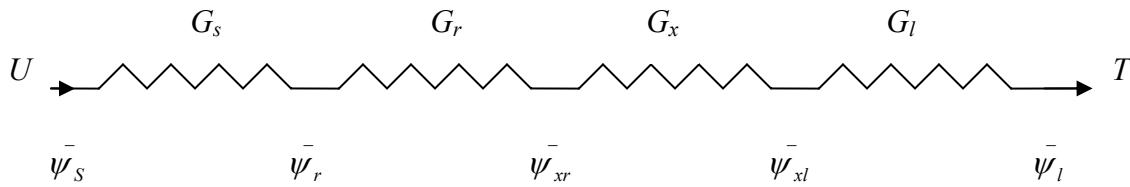
Figure 3. Analog scheme of the soil plant atmosphere continuum showing water potentials and conductances.

The term U refers to the liquid water uptake by roots and T is the water vapor loss as transpiration from the leaves (kg m^{-2}h^{-1}), G_s, G_r, G_x and G_l are the hydraulic conductance (kg^{-2}m^{-2}J^{-1}h^{-1}) of the soil, root, xylem and leaf, respectively, and $\bar{\psi}_s, \bar{\psi}_r, \bar{\psi}_{xr}, \bar{\psi}_{xl}$ and $\bar{\psi}_l$ are the respective average water potential (J kg^{-1}).

If an overall plant conductance (G_p) is defined as the series combination of all conductances, then:

$$T = \left(\overline{\psi}_s - \overline{\psi}_l \right) G_p \tag{86}$$

2.4.1. Root water uptake

The maximum value of G_p (G_{pmax}) can be determined if a maximum uptake rate (U_{max}) is known or assumed for a crop fully shading the soil and well supplied with water. Under this set of conditions, any evaporative demand larger than the maximum uptake rate will induce stomatal closure (Jara, 1995).

$$G_{p\,max} = \frac{U_{max}}{(\psi_{fc} - \psi_{l,onset})} \tag{87}$$

where ψ_{fc} is the soil water potential at field capacity (-33 J kg^{-1}) and $\psi_{l,onset}$ is the leaf water potential (J kg^{-1}) at the onset of water deficit-induced stomatal closure (Stöckle and Jara, 1998). The value of G_p increases as the crop develops, reaching the value of $G_{p\,max}$ when the crop shades completely the soil surface. Thus, the value of G_p is equal to:

$$G_p = G_{p\,max}\ f_{int} \tag{88}$$

where f_{int} is the fraction of solar interception by the crop.

If it is assumed that G_s and G_x conductances are large compared to G_r and G_l (i.e water uptake is not limited by water movements towards the root and through xylem), the partition of plant conductance between the two remaining terms can be approximated as (Campbell, 1985):

$$G_r = \frac{G_p}{0.65} \tag{89}$$

$$G_l = \frac{G_p}{0.35} \tag{90}$$

where G_r and G_l are the roots and leaf hydraulic conductances.

On the other hand, the total water uptake that is equated to transpiration (i.e., plant water storage is assumed negligible) is the sum of the water uptake from each soil layer:

$$U_i = G_{pi}(\psi_{si} - \bar{\psi}_l) \tag{91}$$

where $\bar{\psi}_l$ is the mean leaf water potential (J kg^{-1}), index i refers to the soil layer number, G_{pi} is the layer plant hydraulic conductance and ψ_{si} is the soil layer water potential (J kg^{-1}) determined as (Campbell, 1985):

$$\psi_{si} = \psi_e\left(\frac{\theta_i}{\theta_{si}}\right)^{-b} \tag{92}$$

where ψ_e is the air entry water potential (J kg^{-1}) (potential at which the largest water filled porous just drain), and b is a fitted parameter. The terms θ_i and θ_{si} are the current and saturation volumetric water content, respectively.

The volumetric water content after uptake for a layer is determined as follows:

$$\theta_i^j = \theta_i^{j-1} - \frac{U_i^{j-1}}{z_i \rho_w} \tag{93}$$

where super index j reflects the time step, z_i is the layer thickness (m) and ρ_w is the water density (kg m^{-3}).

The layer plant hydraulic conductance is given by:

$$G_{pi} = \frac{G_{ri} G_{li}}{G_{ri} + G_{li}} \tag{94}$$

where G_{ri} and G_{li} are the apparent hydraulic root and leaf conductance for a particular soil layer. The root hydraulic conductance in each soil layer depends on the fraction of roots present in the

layer and their activity. The model assumes that G_{ri} is equal to G_r weighted for two factors

varying from 0 to 1; the root activity factor f_{ai} and the root fraction f_{ri} as:

$$G_{ri} = G_r f_{ai} f_{ri} \tag{95}$$

where f_{ai} accounts for the root activity as a function of the layer soil water potential (ψ_{si}) and is

given by:

$$f_{ai} = 1 - \left(\frac{\psi_{si} - \psi_{fci}}{\psi_{lwi} - \psi_{fci}} \right)^n \tag{96}$$

where ψ_{fci} is the soil water potential at soil field capacity, ψ_{lw} is the leaf water potential at the

plant wilting point (full stomatal closure), and n is a coefficient (n = 8). The fraction of roots in

each layer is calculated assuming a linear decrease of root density from a maximum in the top

layer to a value of zero at the tip of the root system. Defining R_d (m) as the root depth, d_z (m) as

the layer thickness, and z (m) as the layer bottom depth, then root fraction per layer is computed

as:

$$\text{if } R_d > z_i \text{ then } f_{ri} = d_{zi} \frac{2(R_d - z_i) + d_{zi}}{R_d^2} \tag{97}$$

$$\text{if } R_d < (z_i - d_{zi} + 0.0001) \text{ then } f_{ri} = 0 \tag{98}$$

$$\text{if } R_d = z_i \text{ then } f_{ri} = \left(\frac{R_d - z_i + d_{zi}}{R_d} \right)^2 \tag{99}$$

The average soil water potential $(\bar{\psi}_s)$ is calculated as follows :

$$\bar{\psi}_s = \sum \psi_{si} \left(\frac{f_{ai} f_{ri}}{\sum f_{ai} f_{ri}} \right) \tag{100}$$

It is assumed that the layer apparent leaf water conductance varies in the same proportion as G_{ri}, subsequently:

$$G_{li} = G_l \left(\frac{f_{ai} f_{ri}}{\sum f_{ai} f_{ri}} \right)$$ (101)

Because T is assumed equal to water uptake, the following relations apply:

$$\bar{\psi}_x = \bar{\psi}_s - \frac{T}{G_r}$$ (102)

and

$$\bar{\psi}_l = \bar{\psi}_x - \frac{T}{G_l}$$ (103)

where $\bar{\psi}_x$ is the mean xylem water potential (J kg^{-1}), and T (kg m^{-2}h^{-1}) is the total transpiration (sunlit plus shaded leaves) and $\bar{\psi}_l$ (see equation 91) is the mean leaf water potential.

To determine the mean leaf water potential of sunlit and shaded canopy fractions, $\bar{\psi}_x$ from Eq. (102) is calculated using the total transpiration, and then is prorated between sunlit and shaded canopy fractions so that Eq. (103) is applied using T and G_l for the corresponding fraction: which allows T equilibrates with U as follows:

$$\bar{\psi}_{ls} = \bar{\psi}_x - \frac{T_s}{G_{ls}}$$ (104)

where subindex s is for sunlit or shaded quantities. The prorated G_l (G_{ls}) is computed as follows:

$$G_{ls} = \frac{G_l}{l_{cf}}$$ (105)

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where l_{cf} is the leaf conductance fraction, which has individual values for sunlit and shaded fractions computed as:

$$l_{cf} = \left(\frac{LAI_s}{LAI} + \frac{T_s}{T} \right) 0.5 \tag{106}$$

2.5. Iterative solution

Coupled equations involving the assessment of canopy transpiration, leaf and canopy temperature, photosynthesis, stomatal conductance, and plant water uptake are solved through a nested numerical procedure for the sunlit and shaded canopy fractions. Figure 4 shows a diagram with the main equations and where iterative solutions are performed.

2.6. Parameterization of the model for wheat and maize

The values of model parameters used for the simulation of wheat and maize transpiration and photosynthesis, and corresponding references, are given in Table 2. Data of g_s versus D_l coming from literature were fitted to a hyperbolic function to vapor pressure deficit to define g_{Dl}^0 and D_o (Eq. 79) while data for g_s versus mean leaf water potential data $\left(\bar{\psi_l} \right)$ were fitted to Eq. (85) to define $\psi_{l,onset,}$ $\psi_{1/2}$ and n. On the other hand, the set of equations to asses CO_2 uptake in C_3 and C_4 assimilation pathway, presented in sections 2.3.1.1. and 2.3.1.2., were fitted to data from literature to identify V_m, K_c and K_o in C_3 plants and V_m and u in C_4 plants.
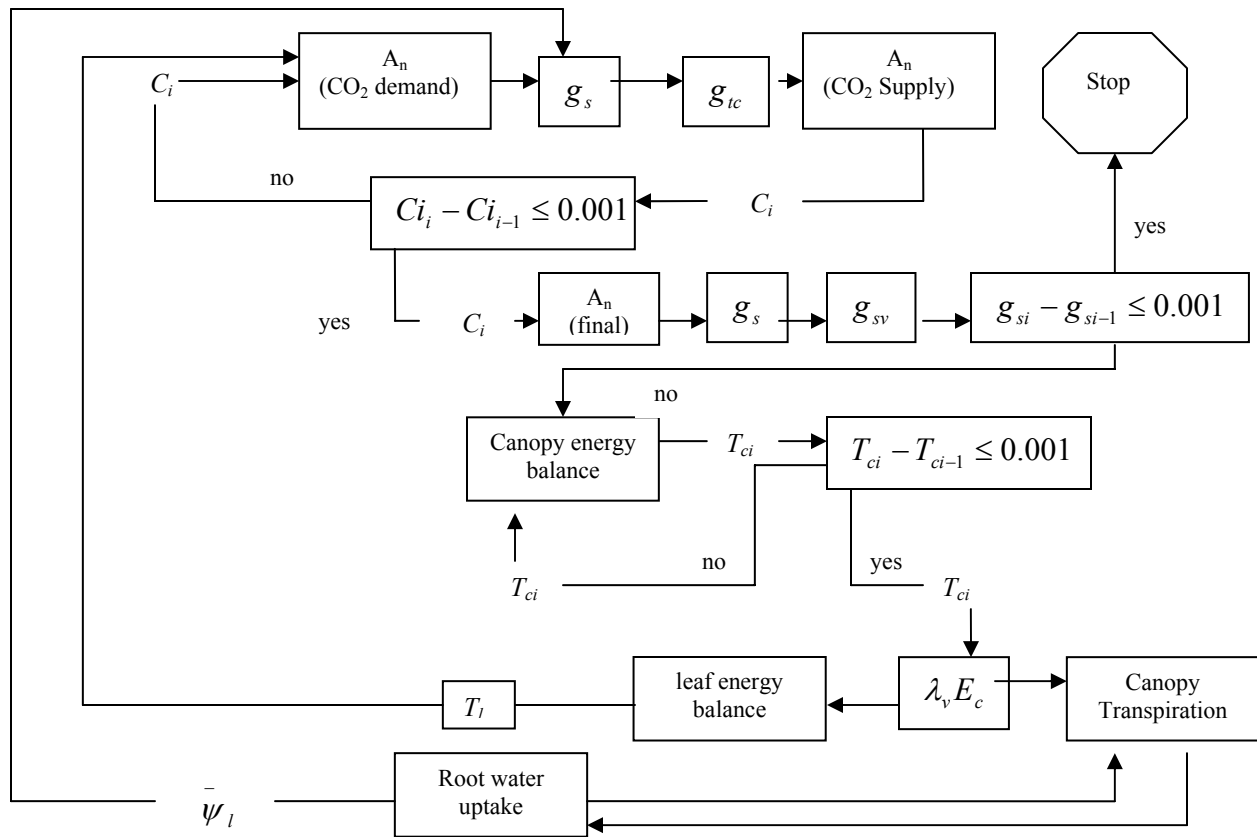
Figure 4. Model diagram of main equations and their iterative solution. Where A_n is the leaf net photosynthesis, T_c and T_l are canopy and leaf temperature, g_s, g_{tc}, g_{sv} are the average leaf stomatal conductance for CO_2, leaf conductance to CO_2 and water vapor, $\bar{\psi}_l$ is the average leaf water potential, $\lambda_v E_c$ is the canopy latent heat, i is and index indicating time step, and C_i is the internal CO_2.

Table 2. List of the parameters used by the model with their respective source.

parameters	Maize	Source	Wheat	Source
$CO_{2\ current}$ (umol mol^{-1})	365		365	
f_{abg}	0.33	(39,41)	0.33	(39,41)
K_c			237.571	(16,27)
K_o			328.854	(16,27)
δ			0.08	(8)
θ	0.783	(30)	0.7	(16,27)
β	0.7	(30)	0.731	(16,27)
V_m	51.514	(30)	135.649	(16,27)
u	1.038	(30)		
$\delta\gamma$	0.067	(9)		
g_{Dl}^{0}	0.871	(13, 45)	2.308	(65)
D_o	0.667	(13,45)	0.402	(65)
fad	0.5		0.5	
fab	0.5		0.5	
$g_s^{max\ *1}$	0.5	(31,32,33,46,48,53,55)	0.5	(3,5,16,24,27,32,33,43,65)
$CO2_{atm}$ (umol mol^{-1})	365		365	
PAR	2000		2000	
T_{leaf}	32		28	
x	1	(6)	0.96	(6)
L_w	0.1		0.02	
h_{cmax}	2.5		1	
LAI_{max}	6		6	
$\Psi_{l,onset}$	-1100	(1)	-1300	(19,27)
$\Psi_{l,w}$	-2500	(1)	-3000	(19,27)
$T_{p,onset}^{*2}$	1.2		1	
$\Psi_{1/2}$	-1662.8	(1)	-1603	(19,27)
n	7.09	(1)	21.268	(19,27)
z	1		1	
d_z	0.1		0.1	
d_n	10		10	
ψ_e	-5		-5	
b	3.8		3.8	

ψ_{fci}	-33	-33
ψ_{pwp}	-1500	-1500
ρ_b	1.4	1.4
wc	0.287	0.287
wp	0.105	0.105
L_w	0.1	0.02

[1]: maximal leaf stomatal conductance to CO_2, described as the seasonal maximum leaf conductance achieved in the field for unstressed, well-illuminated leaves which are fully developed but not senescent (Körner, 1994).

[2]: full cover transpiration rate at the onset of stomatal closure (mm hr^{-1}).

2.7. Model evaluation

2.7.1. Field data

The model was evaluated with climatic and crop data from the Conservation and Production Research Laboratory, Bushland, TX ($35^o11'$ N, $102^o06'$ W; elevation 1170m above mean sea level). Crop information including daily *LAI*, evapotranspiration, crop height and biomass production for wheat (*Triticum aestivum*; 1989-1990, 1991-1992 and 1992-1993 growing seasons), and maize (*Zea mays*; 1990 growing season and Pioneer 3245; 1994 growing season) were available. Ideally, biomass data should include both root and shoot mass. However, root dry mass is difficult to measure and was not reported. Crop evapotranspiration was extracted for daily periods between 7 am and 7 pm from lysimetric measurements. These data came from two groups of two adjacent lysimeters identified as North east (NE) and South east (SE) for wheat (1991-1992) and maize (1990); and North west, (NW) and South west (SW) for wheat (1989-1990; 1992-1993). For maize 1994 only a single lysimeter data was utilized (SE). These data were selected because presented a complete climatic and crop information without missing

data. Daily weather data included daily global irradiance, daily mean wind velocity (7am-7pm), maximum and minimum air temperature and relative humidity, recorded by instruments adjacent to each lysimeter, and deployed over the same crop as in the lysimeter.

A shortcoming of the data is that crop transpiration needed to be estimated. For this purpose a simple approach assuming that crop transpiration is proportional to the fraction of solar irradiance intercepted by the foliage was used:

$$T = ET(1 - \tau_{bt}) \tag{107}$$

where T is crop transpiration (kg m^{-2}), ET is the lysimeter evapotranspiration (kg m^{-2}) and τ_{bt} is the fraction of incident solar irradiance that penetrates the canopy and reaches the soil surface. The crops were well watered and no water stress was documented.

2.7.2. Sensitivity analysis

Some of the parameters needed by the model are easily observable and/or have low variability as reported in the literature, and were held constant once they were determined for a given crop or site. Other parameters reported in the literature present significant variability, and they may impact output results depending on the value selected. This group was selected for a sensitivity analysis.

The analysis was performed during the 1992-1993 growing season for wheat (DOY 88 to 117) and the 1990 growing season for maize (DOY 194 to 222), using the meteorological data acquired by the USDA-ARS at Bushland, Texas. The model input parameters included were the following: stomatal conductance parameters ($gs_{Dl}^{0}, D_{o}, g_{s}^{max}$), leaf photosynthesis parameters (V_{m}, K_{c}, u), crop water relations parameters ($\psi_{l,onset}, n$), and canopy parameters (x). The outputs considered for evaluation were transpiration and photosynthesis for the period. The analysis was

carried out for C_3 metabolism except for the leaf photosynthesis parameters analysis that

included C_4 metabolism as well. Model output sensitivity to a given input (S_e) was obtained as

the ratio between the change in the model output (ΔO) for a given change in the input (ΔI) as:

$$S_e = \frac{\Delta O}{\Delta I} = \frac{\dfrac{(O - O_o)}{O_o}}{\dfrac{(I - I_o)}{I_o}} \tag{108}$$

where I_o is the original value of the input and O_o is its corresponding model output and I and O

are the new values after a change of input parameter was applied. The selected ΔI was $\pm 50\%$ of

the initial parameter value.

2.7.3. Model performance

Evaluation of model performance was based on agreement of simulations and

observations of crop transpiration. Agreement of the model outputs with field observations was

tested with graphical and statistical methods. Graphical methods give a visual sense, through

inspection, of agreement between the model outputs and observed data, whereas statistical

methods give a numerical quantification of agreement. The Willmott index of agreement (D;

Willmott, 1984) was calculated, the root mean square error (RMSE); the mean absolute error

(MAE; Annandale et al., 2004), and the coefficient of residual mass (CRM; Loague and Green,

1991) were calculated. These statistical indexes have the following expressions:

$$RMSE = \sqrt{\frac{\sum\limits_{i=1}^{n}(Pi - Oi)^2}{n}} \quad \frac{1}{O} \tag{109}$$

$$MAE = \frac{\dfrac{1}{n}\sum\limits_{i=1}^{n} Abs(Pi - Oi)}{O} \tag{110}$$

$$D = 1 - \frac{\sum\limits_{i=1}^{n}(Pi - Oi)^2}{\sum\limits_{i=1}^{n}(|Pi - O| + |Oi - O|)^2} \tag{111}$$

$$CRM = \left(\sum\limits_{i=1}^{n} Oi - \sum\limits_{i=1}^{n} Pi\right) \bigg/ \sum\limits_{i=1}^{n} Oi \tag{112}$$

where Pi and Oi are predicted and observed values of transpiration or photosynthesis; n is the number of pairs of data, and O is the mean of the observations. The optimal "accuracy" is achieved when RMSE, MAE and CRM are equal to zero and D is equal to one. Positive values of CRM indicate model underestimation, while negative indicate overestimation.

3. RESULTS AND DISCUSSION

3.1. Sensitivity Analysis

The results of the analysis are presented in Tables 3 and 4. Values of S_e were less than one, which is an indication of model robustness. The S_e coefficients obtained were always 0.577 or less implying that for a given error in the input, the error generated in the output is proportionally lower, and therefore, errors are not magnified by the model. Canopy transpiration estimations seems to be more sensitive to g_s^{max}, with S_e absolute values up to 0.577, followed by V_m (C$_3$: 0.273 and C$_4$: 0.286) and g_{Dl}^0 (0.207). The sensitivity to g_s^{max} was expected since it works as a "buffer" reducing the effects of the g_s vs D_l fitted curve when the crop is grown under low D_a atmospheric conditions. Error in other parameters had a relatively small influence on the estimated transpiration. Photosynthesis seems to have a low sensitivity to all the parameters tested but V_m, which showed S_e values of 0.383 in C$_3$ and 0.526 in C$_4$ plants.

Table 3. Sensitivity of canopy transpiration outputs to changes of selected inputs (-50% and $+50\%$ respectively).

Input parameters Stomatal conductance	-50%	+50%	Overall
g_{Dl}^{0}	0.207	0.004	0.106
D_o	0.117	0.004	0.061
g_s^{max}	0.577	0.332	0.455
Leaf photosynthesis C3			
V_m	-0.273	-0.168	0.221
K_c	0.114	0.102	0.108
Leaf photosynthesis C4			
V_m	-0.286	-0.108	0.197
u	-0.031	0.114	0.073
Crop water relations			
$\psi_{l,onset}$	-0.019	-0.164	0.092
n	0.024	0.006	0.015
Canopy			
x	-0.065	-0.056	0.061

Table 4. Sensitivity of photosynthesis outputs to changes of selected inputs (-50% and $+50\%$ respectively).

Input parameters			
Stomatal conductance	**-50%**	**+50%**	**Overall**
g_{Dl}^{0}	0.026	0.001	0.014
D_o	0.016	0.001	0.009
g_s^{max}	0.081	0.013	0.047
Leaf photosynthesis C3			
V_m	0.383	0.154	0.269
K_c	-0.087	-0.082	0.085
Leaf photosynthesis C4			
V_m	0.526	0.211	0.44
u	0.083	-0.087	0.085
Crop water relations			
$\psi_{l,onset}$	-0.001	-0.012	0.007
n	0	0	0
Canopy			
x	-0.208	-0.138	0.173

3.2. Model performance

3.2.1. Canopy transpiration

Daily simulated and observed canopy transpiration is presented in Figures 5, 6 and 7 for wheat and maize simulations. The data presented were selected to represent middle stage of vegetative growth, which involves the period after the crop reach a green *LA*I of 2.5 and just days after the beginning of canopy senescence. The figures show a good agreement between simulated and observed canopy transpiration, with the model tracking well the daily fluctuations. The good performance of the model is also supported by the statistical indices (Table 5). The RMSE, MAE and D for wheat ranged from 0.17 to 0.26, 0.13 to 0.20 and 0.90 to 0.93, respectively; whereas for maize these indices ranged from 0.11 to 0.18, 0.09 to 0.16 and 0.90 to 0.93, respectively. There was a slight tendency to underestimate transpiration for wheat and maize, results supported by the sign of the of CRM index (Table 5).

Table 5. Statistical indexes of agreement between observed and simulated canopy transpiration of wheat and maize growth in Bushland, Texas.

Crop	RMSE	MAE	D	CRM
wheat 1989-1990NE	0.226	0.176	0.926	-0.080
wheat 1991-1992NE	0.190	0.143	0.919	0.104
wheat 1991-1992SE	0.148	0.117	0.918	0.012
wheat 1992-1993NW	0.173	0.142	0.931	0.096
wheat 1992-1993SW	0.191	0.159	0.919	0.089
maize 1990NE	0.130	0.111	0.941	-0.090
maize 1990SE	0.107	0.084	0.923	0.023
maize 1994SE	0.143	0.124	0.904	0.088
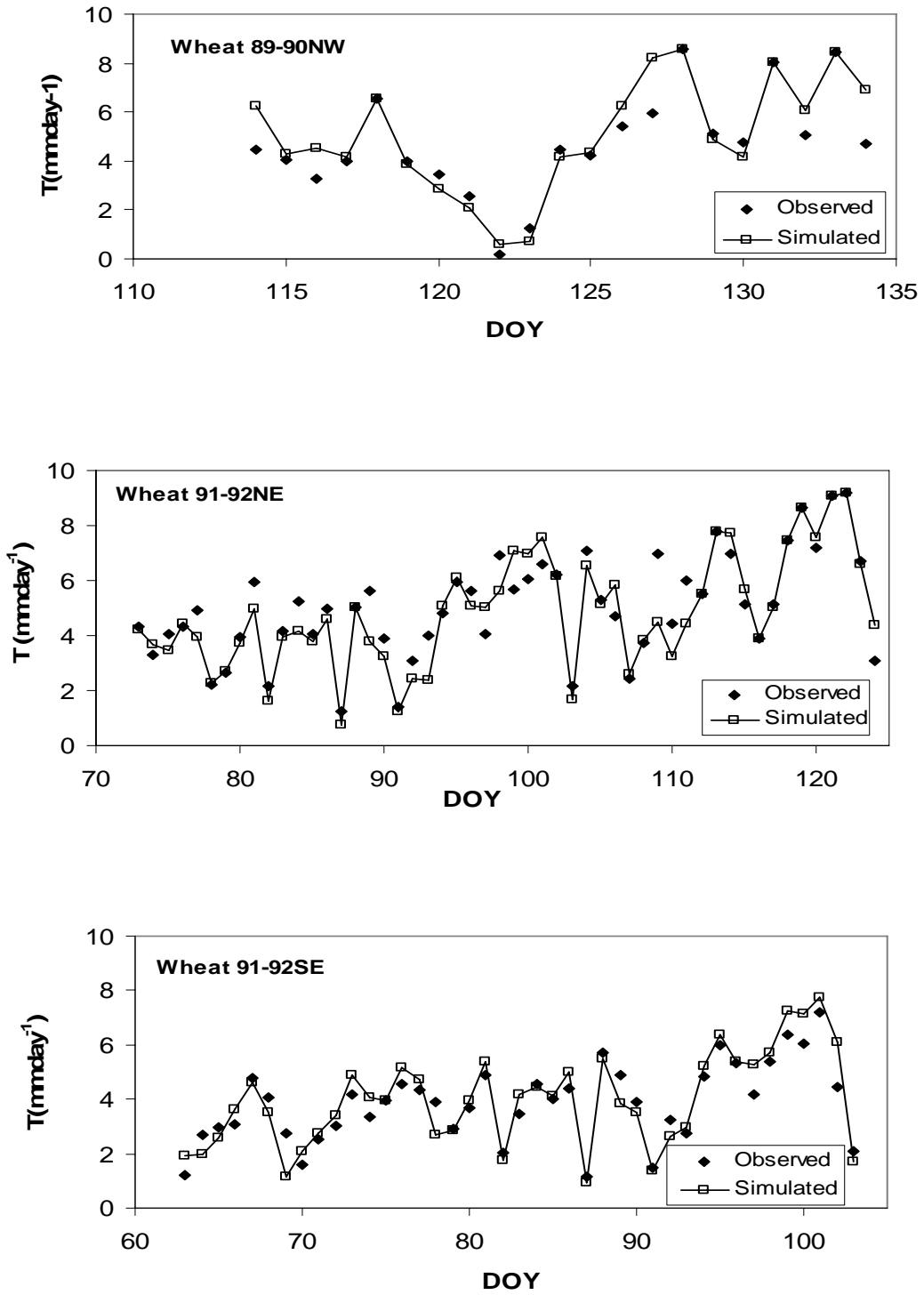
Figure 5. Daily measured and simulated crops transpiration values in wheat.
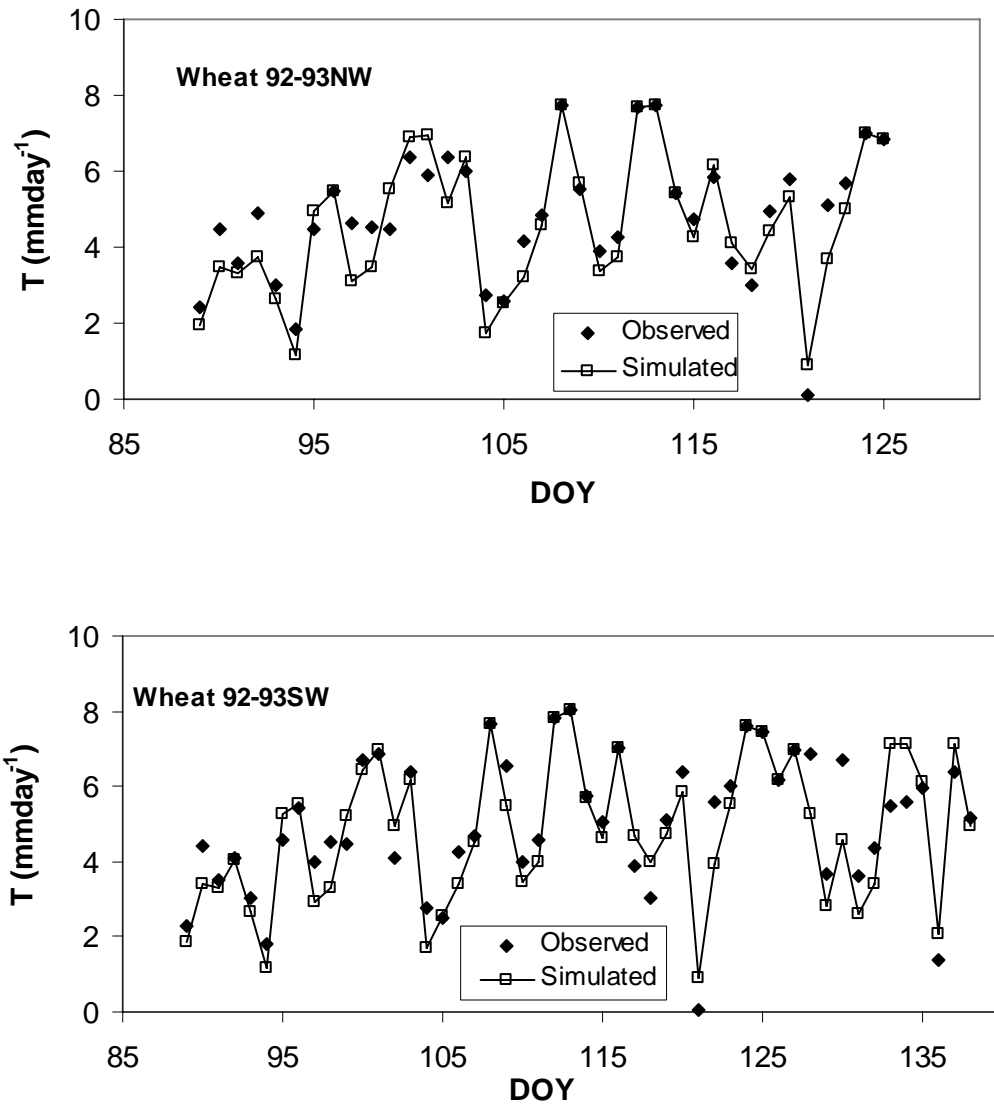
Figure 6. Daily measured and simulated crops transpiration values in wheat.
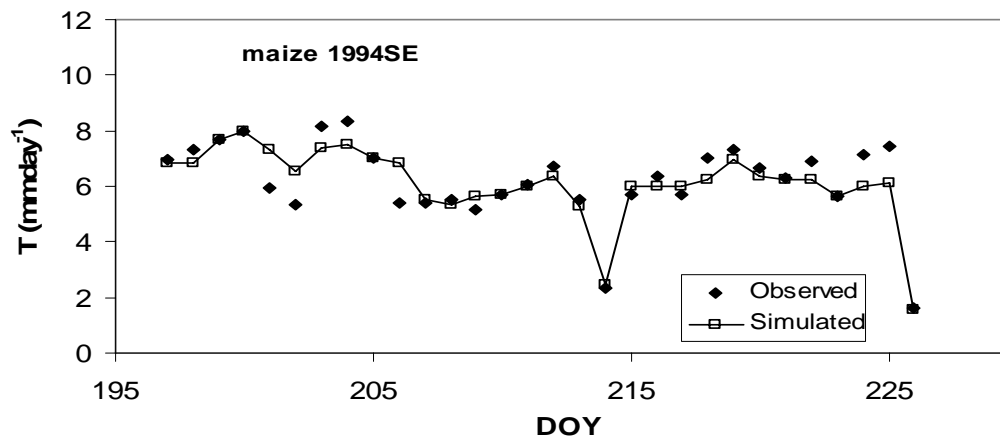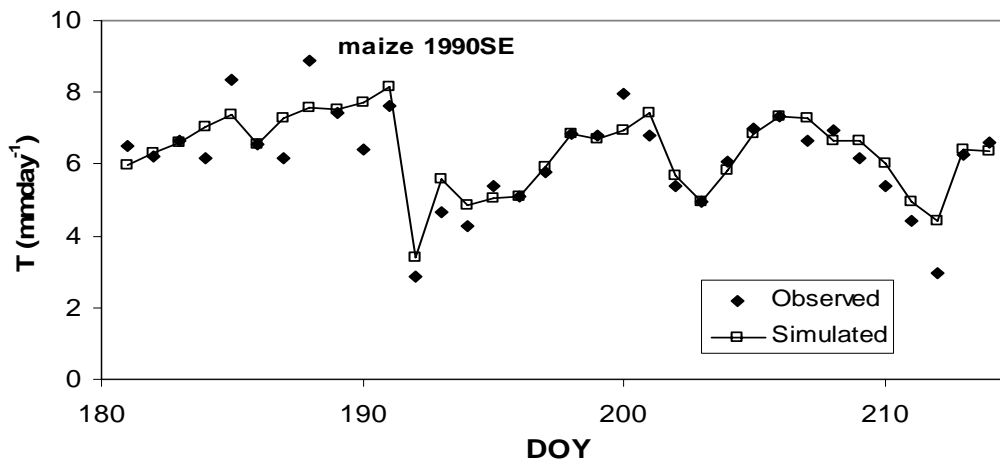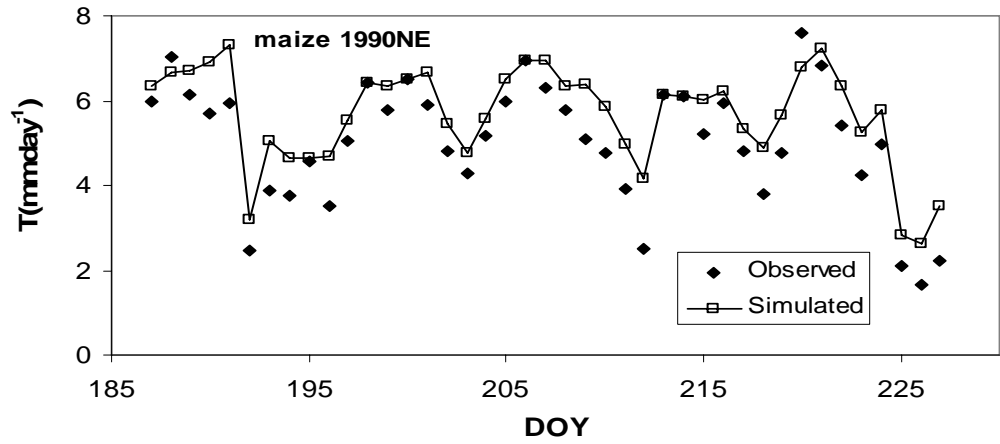
Figure 7. Daily observed and simulated crop transpiration values in maize.

One to one plots comparing observed and simulated transpiration for wheat and maize are shown in Figures 8 and 9. A linear regression, forced through the origin, resulted in a slope of 0.98 (r^2=0.85) for wheat and 1.03 (r^2=0.64) for maize. Four sources of error could explain some of the differences: (1) parameters are not specific for the varieties tested, (2) field measurement errors, (3) accuracy in the methodology used to transform the evapotranspiration data from lysimetric measurements to transpiration, and (4) inaccuracies arising from the transformation of daily to hourly weather data.
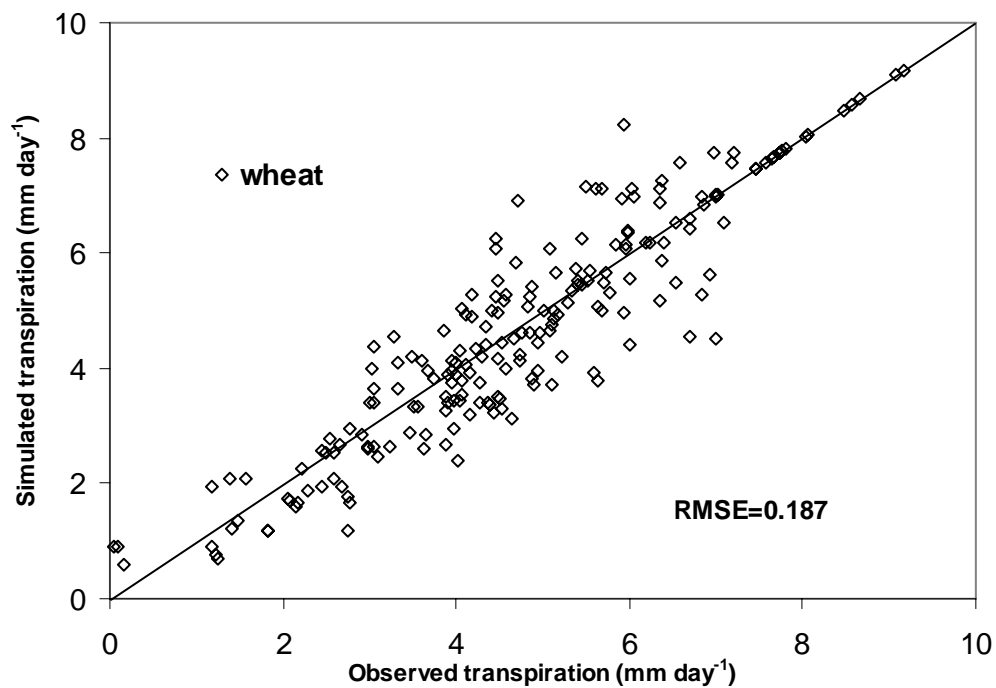
Figure 8. Comparison of observed and simulated canopy transpiration for wheat.
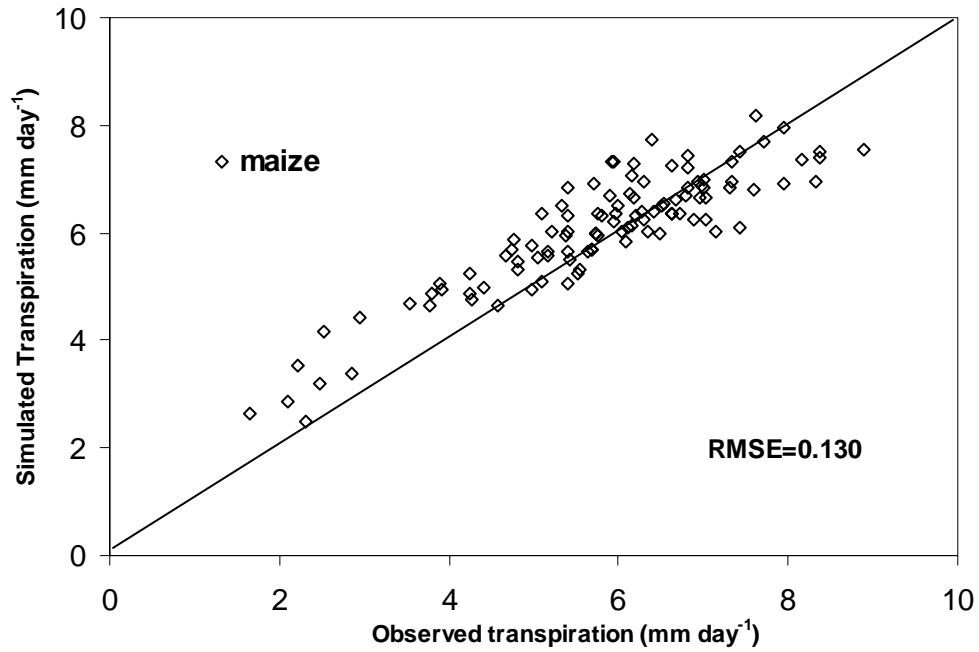
Figure 9. Comparison of observed and simulated canopy transpiration for maize.

3.2.2. Transpiration-use efficiency

The model calculates transpiration–use efficiency (w) as kg of CO_2 fixation per kg of water transpired. This information cannot be compared directly with the available data from literature, which usually includes above ground biomass production and transpiration. In order to express w as kg of biomass per kg of water transpired it is necessary to transform photosynthesis to biomass production. Monteith (1981) suggested that: 1) the fraction of photosynthesis loss by growth and maintenance respiration (f_r) is often near 0.4, and 2) biomass produced by a crop can be assumed a constant fraction of photosynthesis. Therefore, as a first approximation, the following factor times photosynthesis would estimate biomass production:

$$f_{DM} = 0.682(1 - f_r) \tag{113}$$

where 0.682 is the ratio of molecular weights of CH_2O and CO_2. To estimate aboveground biomass the fraction of biomass apportioned to the roots has to be discounted. Thus, the conversion factor of mass of CO_2 fixation to aboveground biomass is given by:

$$f_{abg} = \frac{0.682(1 - f_r)}{(1 + r)} \tag{114}$$

where r is the root to shoot fraction. Considering a mean r value for wheat and maize of 0.25 (Lorenz and Lal, 2005), f_{abg} should be near 0.33.

Daily simulated values of transpiration–use efficiency were transformed to aboveground w using f_{abg}, and compared with w values obtained from literature in both crops; results are shown in Table 6. These results indicate that the average and standard deviation of the simulated results are within the range of the observed data; hence, despite the variability of the observations due to varieties, methods to determine transpiration, biomass sampling and experimental error, the agreement appears encouraging.

Table 6. Number of data (n), mean (x), and standard deviation (s) from daily simulated w (g kg^{-1}) values and observed w (g kg^{-1}) values.

Crop	simulated			Observed[1]		
	n	x	s	n	x	s
wheat	201	4.29	2.07	36	4.90	1.34
maize	108	5.65	1.02	14	5.82	1.18

[1]: to see sources of observed data refers to chapter 3.

4. CONCLUSIONS

The CTP model showed to be a reliable tool that requires relatively easy–to–obtain input parameters and offers a wide range of applicability including different crops and weather conditions.

Sensitivity analysis indicated that canopy transpiration and photosynthesis simulation outputs were not sensitive to changes of most input parameters, having its highest sensitivity to g_s^{max} in the case of canopy transpiration estimation, and to V_m in the case of photosynthesis estimation. However, the overall values of the sensitivity coefficients obtained were always 0.58 or less, indicating a maximum relative change of output of 0.58 for a given unit change of input, with most values lower than this, which is and indication of model robustness.

Model simulations of transpiration, tested against field data in wheat and maize, showed good agreement with the time evolution of the observed data. This was confirmed with values of RMSE, MAE and D for both crops less than 0.26 and 0.20, and higher than 0.91, respectively, with a slight tendency to underestimate transpiration for both crops. Four sources of error could explain some of the differences: (1) parameters are not specific for the varieties tested, (2) field measurement errors, (3) accuracy in the methodology used to transform the evapotranspiration data from lysimetric measurements to transpiration, and (4) inaccuracies in the transformation of daily to hourly weather data.

The model calculates transpiration–use efficiency (w) as kg of CO_2 fixation per kg of water transpired. This information was converted to w (kg of aboveground biomass per kg of water transpired) using a conversion factor (f_{abg}) and compared with observed data from different locations as a function of air vapor pressure deficit for wheat and maize. Despite,

differences in cultivars, crop management, methods to estimate transpiration, sampling methods for biomass, and other sources of variability and experimental error of the available observed data, the agreement appeared adequate in terms of mean and standard deviation of simulated and observed data.

Further model evaluation with a larger variety of crops and weather conditions should be performed. The inclusion of routines to deal with fruit trees orchards and the effect of different irrigation techniques in crop-soil water relationships may broaden the range of application of this model.

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CHAPTER TWO

Evaluating the Transferability of Simple Transpiration–Use Efficiency models of Biomass Production

ABSTRACT

Transpiration–use efficiency, defined as the ratio of biomass (B) produced per unit of water transpired (T), has been used to evaluate crop productivity as a function of water supply. Plots of biomass production vs. transpiration usually show a linear relation, with the scatter around the regression line decreasing when transpiration is normalized by atmospheric evaporative demand described either by atmospheric vapor pressure deficit (D_a), pan evaporation, or reference crop evapotranspiration (ET_o). Thus, simple approaches to assess transpiration–use efficiency (w) have been proposed including: 1) $w = k_{Da}/D_a$ and 2) $w = k_{ETo}/ET_o$; where k_{Da} and k_{ETo} are crop–dependent parameters. The underlying concept in these approaches is that normalization by D_a or ET_o accounts for the effects of climate variations on w, while k_{Da} or k_{ETo} are expected to be reasonably constant across diverse climatic conditions. Experimentally, these parameters can be determined as the slope of the regression between cumulative biomass and the daily accumulation of T/Da or T/ET_o. The transferability of experimentally–determined parameters across locations with diverse climate is important, allowing a wider application of these parameters for the estimation of crop productivity. The objective of this study was to evaluate the transferability of k_{Da} and k_{ETo} values for wheat and maize across world locations with contrasting climate. The evaluation of the transferability of

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these parameters is not simple due to the scarcity of experimental information and the lack of

consistency of the methodology used in the available experiments. For this reason, a canopy

transpiration and photosynthesis (CTP) model was developed, tested, and used to simulate values

of k_{Da} and k_{ETo}, with the advantage that these values are obtained with a consistent

methodology. Weather data from eight environmentally different locations were used for these

simulations. The results indicated that w, k_{Da} and k_{ETo} are not constant, suggesting that

calibration in contrasting climates would be desirable. However, a consistent trend of change of

the values of the parameters as a function of D_a or ET_o was found, which can be represented by

mathematical functions, allowing the possibility of transferring w, k_{Da} and k_{ETo} (maize) values

across climatic conditions. On the other hand, the k_{ETo} for wheat correlated weakly with D_a and

ET_o, but a low overall coefficient of variation (10%) of this parameter across the eight locations

allowed the use of an average k_{ETo} value as a reasonable predictor of w, regardless of climatic

conditions. Verification of the simulation-based equations presented here with field data will be

needed before its use for wheat and maize (and perhaps similar C_3 and C_4 species) can be

recommended.

1. INTRODUCTION

Agriculture is challenged by the scarcity of water resources in many regions of the world, problem that is compounded by climate variability and expected to worsen in the future. There is a raising need for tools to evaluate crop productivity as a function of water to better guide development policies and field management practices aimed at producing "more crop per drop".

Mechanistic simulation models of canopy photosynthesis and transpiration appear as suitable tools to evaluate the effect of interacting factors on water–use efficiency and productivity of crops. However, demanding parameterization and computing requirements of these models limit their applicability for long–term analysis that includes multiple species across the globe (eg. Sinclair et al., 1976; Leuning et al., 1995).

Simple models based on transpiration–use efficiency (*w*), able to evaluate biomass production in response to water using a few parameters, are an attractive alternative. Attempts to develop simple relationships to predict transpiration–use efficiency for different crops and climates can be traced back to the early 20th century and later (eg. Brigss and Shantz, 1913a, 1913b, 1914; Shantz and Piemeisel, 1927; de Witt, 1958; Arkley, 1963, 1982; Bierhuizen and Slatyer, 1965; Tanner, 1981; Ritchie, 1983; Tanner and Sinclair, 1983; Steduto and Albrizio, 2005). The underlying assumption has been that the parameters of these relationships are relatively constant across diverse climatic conditions, and assumption that has not been well evaluated.

Early work by Bierhuizen and Slatyer (1965) led the way to the development of a comprehensive physiologically–based description of transpiration use efficiency as follows:

$$\frac{N_l}{T_l} = \frac{\Delta C / r_{CO2}}{(\rho \varepsilon / P_a) D_l / r_v} \tag{1}$$

where N_l is the net leaf photosynthesis, T_l is the leaf transpiration, ΔC is the CO_2 concentration

difference between the atmosphere and the CO_2 compensation point, r_{CO2} is the leaf resistance to

CO_2 diffusion from the surrounding air into the leaf and into the cells of the chloroplasts, ρ is

the density of the air, ε is the vapor to air molecular weight ratio, D_l is the vapor pressure

difference between the leaf and the surrounding air, P_a is the atmospheric pressure and r_v is the

summation of the partial resistances to water vapor flux from the leaf. Bierhuizen and Slatyer

(1965) showed that the ratio N_l/T_l is determined largely by D_l based on the following

assumptions: (1) ΔC is a relatively constant crop–dependent parameter, and (2) the r_v/r_{CO2} ratio is

fairly constant in active leaves when the water stress is not severe. The authors redefined Eq. (1)

in a simpler expression:

$$\frac{N_l}{T_l} = \frac{k_l}{D_l} \tag{2}$$

where:

$$k_l = \frac{P_a \, \Delta C \, r_v}{\rho \, \varepsilon \, r_{CO2}} \tag{3}$$

here k_l is consider constant for leaves in a given crop. The authors also argued that N_l/T_l should

be proportional to canopy B/T (where B is canopy dry matter and T is canopy transpiration) and,

therefore, k_l could be scaled up to the entire canopy k_{Da} and that D_l could be well represented by

the air vapor pressure deficit D_a since the leaf temperature appear to be within ± 2–$3^{\circ}C$ of air

temperature. Hence:

$$w = \frac{B}{T} = \frac{k_{Da}}{D_a} \tag{4}$$

where k_{Da} is obtained experimentally as the slope of the linear regression between cumulative

biomass and the daily integration of the quotient T/D_a.

Tanner and Sinclair (1983) extended the work initiated by Bierhuizen and Slatyer (1965) and Tanner (1981), developing equations to represent biomass production and transpiration of the sunlit and shaded fractions of the canopy, essentially leading to a re–derivation of Eq. (4).

Although Eq. (4) has been adopted as a reasonable predictor of biomass accumulation (e.g. Stöckle et al., 1994; Sinclair and Seligman, 1995), concerns have been raised about the transferability of k_{Da} (Kemanian et al., 2005). These authors argued that k_{Da} is not a "constant" for a crop, but it rather changes with environmental conditions, most noticeable D_a.

Steduto and Albrizio (2005) presented field data and a discussion of the concept and mechanism of determination of k_{Da}, including C_3 (chickpea, sunflower, wheat) and C_4 (sorghum) species in one location (Bari, Italy; 41° 03'N, 16° 52'E, 72 m above sea level). They found that their k_{Da} values had large variability among species and did not match data for the same species from literature. Two explanations to their findings were mentioned: 1) the error introduced by scaling D_l to D_a, especially in low D_a conditions where leaf temperature can be several degrees larger than air temperature and 2) the effectiveness of D_a normalization to represent D_l since the latter is defined by the transpiration flux, which changes as the physiological stage of the crop changes. They proposed an alternative methodology, similar to the original work by de Witt (1958), where w is a function of the evaporation rate of a reference condition as:

$$w = \frac{B}{T} = \frac{k_{ETo}}{ET_o} \tag{5}$$

where ET_o is the reference crop evaporation computed as proposed by Allen et al. (1998) and k_{ETo} is the slope of the linear regression between cumulative biomass and cumulative (T/ETo). Steduto and Albrizio (2005) claim that this method would work better than Eq. (4) and that k_{ETo}

appeared transferable among different climatic zones. However, this claim was based on limited data and has not been verified.

The main objective of this work was to evaluate the transferability across diverse climatic condition of k_{Da} and k_{ETo} of wheat and maize. However, experimental data allowing the calculation of k_{Da} and k_{ETo} is scarce and does not cover well the wide array of environmental conditions where wheat and maize are grown. In addition, the available data include differences in cultivars, crop management, methods to estimate transpiration, sampling methods for biomass, and other sources of variability and experimental error, making it difficult to evaluate the constancy of the parameters. For that reason, a canopy transpiration and photosynthesis model (CTP, see Chapter 1 for more details) was developed and tested, and used in this chapter as reference to obtain simulated values of w, k_{Da} and k_{ETo} under variable climatic conditions while crop and soil characteristic were held constant, allowing a more consistent evaluation of the transferability of these parameters.

2. MATERIALS AND METHODS

2.1 The model

An hourly time step canopy transpiration and photosynthesis (CTP) model, separating sunlit and shaded fractions of the canopy, was developed to serve as a tool to obtain simulated values of k_{Da} and k_{ETo}. The model simulates carbon assimilation (g CO_2 m^{-2} ground area), and crop transpiration (kg H_2O m^{-2} ground area) in response to climatic conditions, soil and plant water status, and atmospheric CO_2 concentration. Transpiration, photosynthesis, stomatal conductance, and plant water uptake are solved simultaneously through an iterative numerical procedure. Daily measurements of global solar radiation, air temperature, air humidity, and wind speed are inputs to the model. Additional inputs include green plant area index (*LAI*), maximum crop height, maximum *LAI*, assimilation rate as a function of intercellular CO_2 concentration, stomatal conductance response to air vapor pressure deficit and leaf water potential, and soil characteristics (hydraulic parameters, bulk density, depth, and number and thickness of soil layers). Figure 1 and 2 show diagrams depicting the main processes and information flow in the model. Model performance was tested using meteorological and crop data (wheat and maize) collected at the Conservation and Production Research Laboratory, Bushland, TX (35°11' N, 102°06' W; elevation 1170m above mean sea level), indicating the suitability of the model for the application presented in this chapter. A more detailed description of the CTP model and parameters for the simulation of wheat and maize transpiration–use efficiency is presented in a companion chapter (Chapter 1). For this study, soil water content, *LAI*, crop height, and crop parameters for photosynthesis and stomatal conductance were held constant during the entire simulation period at all the locations. Thus, only daily weather was variable.
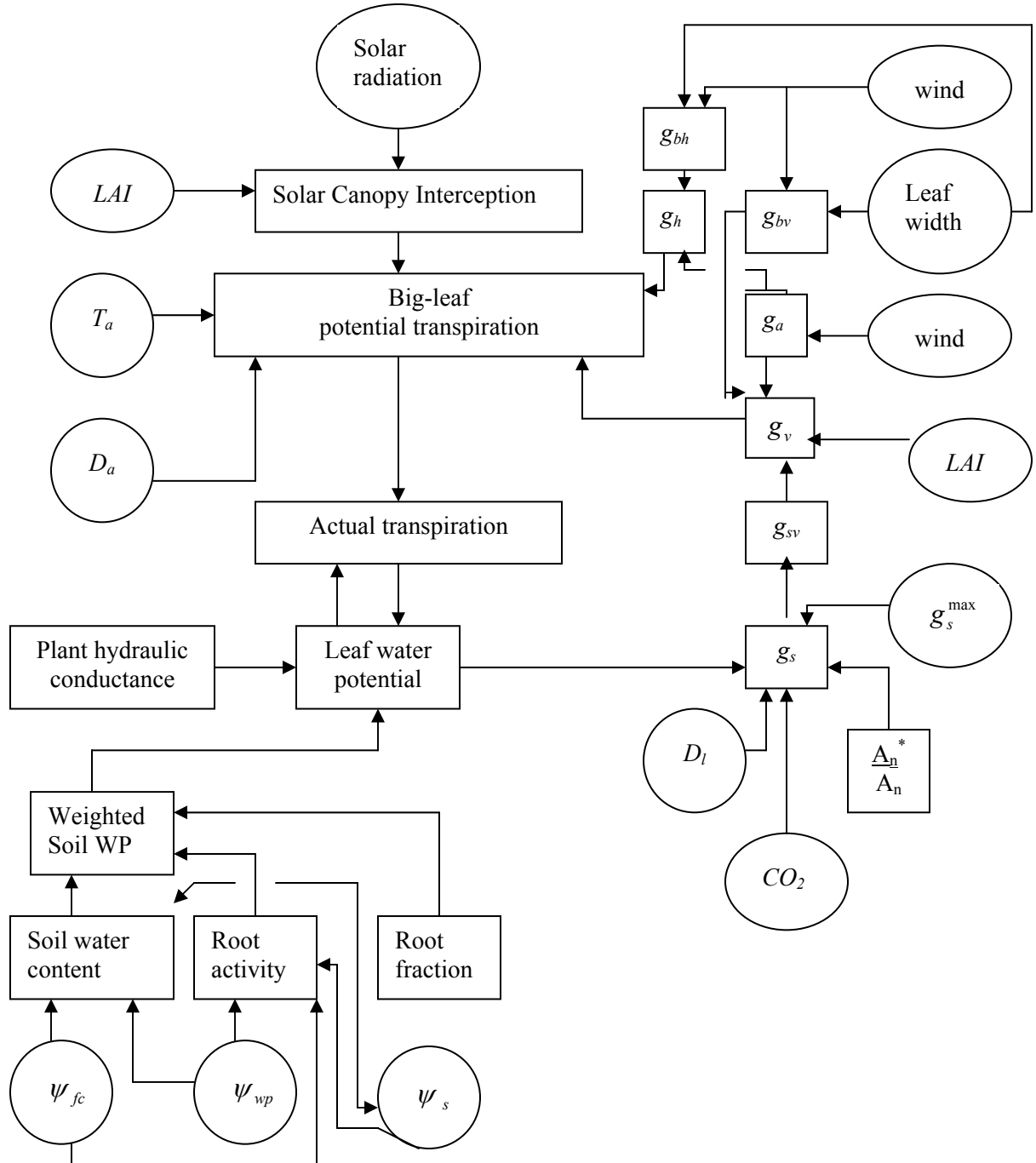
Figure 1. Model diagram for sunlit or shaded leaves transpiration, where A_n* and A_n are reference and current net photosynthesis for an average leaf, T_a and T_l are air and leaf temperature, D_a and D_l are the air and leaf vapor pressure deficit , LAI is the green leaf area index, g_s and g_{sv} are the average leaf stomatal conductance for CO_2 and water vapor, g_a is the aerodynamic conductance, g_h and g_v are the canopy heat and water vapor conductance, g_{bv} and g_{bh} are boundary layer conductance for water vapor and heat, ψ_s is the soil water potential, ψ_{fc}, ψ_{wp} are the soil water potential at field capacity and at wilting point and g_s^{max} is the maximum stomatal conductance to CO_2.

Solar radiation

Leaf solar irradiance

g_{bh}

wind

Leaf PAR Irradiance

Leaf temperature

LAI

Potential photosynthesis (CO_2 demand)

$\lambda_v E_l$

Actual Transpiration

g_a

g_{bc}

Potential photosynthesis (CO_2 supply)

Actual leaf photosynthesis

LAI

CO_2

g_s

$\dfrac{A_n^*}{A_n}$

Leaf Water Potential

D_l

Canopy Photosynthesis

g_s^{max}

f_{DM}

Biomass

Figure 2. Model diagram for sunlit or shaded leaves photosynthesis, where A_n^* and A_n are the reference and current net photosynthesis for an average leaf, D_l is the leaf to air vapor pressure deficit, CO_2 is the atmospheric CO_2 concentration, g_s^{max} is the maximum stomatal conductance to CO_2, g_{bh} and g_{bc} are the heat and CO_2 boundary layer conductance, g_s is stomatal conductance to CO_2 , g_a is the aerodynamic conductance LAI is the green leaf area index, f_{DM} is a conversion factor and $\lambda_v E_l$ is leaf latent heat.

2.2 Meteorological data

To generate a highly diverse set of conditions, daily weather data from eight locations were selected. The data were composed of daily measurements of global solar radiation (MJ $m^{-2}day^{-1}$), maximum and minimum air temperature (^{o}C), maximum and minimum air relative humidity and average wind speed (m s^{-1}), encompassing the period day of the year (DOY) 120 through 239 for a year selected at random in the following locations: Concepcion del Uruguay (Argentina, $32^{o}28'$ S, $58^{o}16'$ W; elevation 20m above sea level), Landriano (Italy, $45^{o}18'$ N, $9^{o}15'$ E; elevation 78m above mean sea level), Temple (TX,USA; 31° 7'N, $97^{o}4'$W; elevation 208m above mean sea level), Pullman (WA,USA, $46^{o}45'$N, $117^{o}1'$W; elevation 756m above mean sea level), Prosser (WA,USA, 46°N, $119^{o}7'$W; elevation 380 m above mean sea level), Ankara (Turkey, $40^{o}7'$N, $32^{o}59'$E; elevation 948m above sea level), Aleppo (Syria, $36^{o}1'$N,$37^{o}18'$E; elevation 430m above sea level) and DOY 166 through 239 for Maricopa (AZ, USA, $33^{o}49'$N, $112^{o}1'$W; elevation 359m above sea level). The main climatic characteristics of the selected period in the eight locations are presented in Table 1.

Table 1. Mean (x) and standard deviation (s) of weather data from eight locations and selected periods.

variables		Concepcion	Landriano	Temple	Pullman	Prosser	Ankara	Aleppo	Maricopa
T_{max}	x	27.8	26	31.2	22.6	27.0	27.9	34.7	38.9
	s	4.0	4.7	3.3	6.8	6.3	6.1	4.9	2.5
T_{min}	x	16.9	14.2	20.6	8.4	9.3	14.3	17.5	24.3
	s	3.3	3.4	2.9	4.2	4.2	4.7	5.3	2.1
S_R	x	21.5	22.5	21.1	23.3	25.7	21.1	27.2	27.6
	s	7.8	6.5	5.8	5.9	5.2	4.4	2.3	3.6
RH_{max}	x	99.7	85.5	92	81.4	61.7	63.1	67.4	78.7
	s	2.2	21.4	6.3	12.4	14.5	14.3	15.0	17.0
RH_{min}	x	64.8	46.7	47.6	32.8	43.4	31.7	25.7	25.1
	s	13.3	21.3	12.9	13.0	9.2	15.3	7.2	11.2
$Wind$	x	3.0	1.2	2.7	2.1	1.5	1.8	4.8	2.2
	s	1.3	0.6	1.1	1.0	0.5	0.7	1.9	0.5
ET_o	x	4.3	4.3	5.3	4.4	4.8	5.0	9.0	7.7
	s	1.5	1.2	1.3	1.2	1.1	1.3	2.0	1.2
D_a	x	0.8	1.0	1.5	1.1	1.3	1.8	2.6	3.2
	s	0.3	0.4	0.6	0.6	0.6	0.8	0.8	0.9

T_{max} and T_{min} are the maximum and minimum air temperatures (^{o}C), S_R is the global solar radiation (MJ m^{-2} day^{-1}), RH_{max} and RH_{min} are the maximum and minimum relative humidity, ET_o is the reference evapotranspiration (mm day^{-1}), and D_a is the day time air vapor pressure deficit (kPa) estimated as: $D_a = 2/3\ e_s\ (T_{max})\ (1-R_{min})$, where $e_s(T_{max})$ is the saturation vapor pressure of the air in kPa at maximum air temperature .

2.3. Determination of k_{Da} and k_{ETo}

Daily transpiration and photosynthesis for wheat and maize were simulated for all locations using the CTP model and assuming well–developed and unstressed crops. The parameters k_{Da} (g CO_2 kg^{-1} H_2O kPa) and k_{ETo} (g CO_2 m^{-2}) were estimated as the slope of the linear regression between cumulative photosynthesis and the accumulation of the transpiration to daytime D_a quotient (eg. Tanner, 1981; Condon et al., 1993) and transpiration to ET_o quotient (eg. Steduto and Albrizio, 2005), respectively. Calculations of the parameters were done for moving 15–day intervals, shifted by 5 days throughout the 120–day period. Daily ET_o calculation were carried out as proposed by Allen et al. (1998).

3. RESULTS AND DISCUSSION

Simulated w values for 15–day periods across eight locations were highly variable (Table 2), with coefficient of variation of 25% and 18% for wheat and maize, respectively, with the implication that w values determined experimentally in one location may not be readily transferable to another. Normalization of w by D_a Eq. (4) or ET_o Eq. (5) is expected to account for weather variability, with the parameters k_{Da} or k_{ETo} remaining reasonable constant. However, as shown in Table 2 k_{Da} and k_{ETo} (maize) present more variability than desirable for transferring values derived in one location to another with k_{Da} variability being greater than that of k_{ETo}.

As pointed out by Tanner (1981) and Steduto and Albrizio (2005), a drawback associated with D_a normalization is usually related to the degree of error introduced on the assumption that D_a is a fair representation of D_l, especially in humid environments. In these environments, transpiration rate is expected to be lower, and as a result leaf temperature should increasingly departs from air temperature making D_l larger than D_a. To test this assumption, the values of k_{Da} obtained in environments with D_a less than 1 kPa were not included in the CV analysis. Some improvement on CV was obtained for both crops however the variability still remained (wheat: 18.75%, and maize: 26.18%).

Figures 3 and 4 present w as a function of the average D_a and ET_o, of each corresponding 15–day interval. Both figures show that w is not constant across environments characterized by D_a and ET_o, and has an important non–linear response to D_a and ET_o (Abbate et al., 2004; Kemanian et al., 2005). Fitted power equations appear good estimators of w, with D_a explaining 94% and 90% of the w variability for wheat and maize, respectively, and ET_o explaining 89%

and 72%, respectively. The dispersion around the fitted lines represents variability due to

climate that is not accounted for by D_a or ET_o. This effect of other weather variables is less

important with D_a and ET_o greater than 2 kPa and 7 mm/day, respectively.

Table 2. Mean (x), standard deviation (s), number of data (n), and coefficient of variation (CV) for simulated w, k_{Da} and k_{ETo} from eight locations.

Parameters		n	x	s	CV %
w (g CO_2 kg^{-1} H_2O)					
	wheat	159	10.71	2.69	25.09
	maize	159	17.50	3.07	17.53
k_{Da} (g CO_2 kg^{-1} H_2O Pa)					
	wheat	159	15.99	4.35	27.21
	maize	159	27.70	9.66	34.88
k_{ETo} (g CO_2 m^{-2})					
	wheat	159	55.87	5.68	10.16
	maize	159	94.37	16.79	17.80

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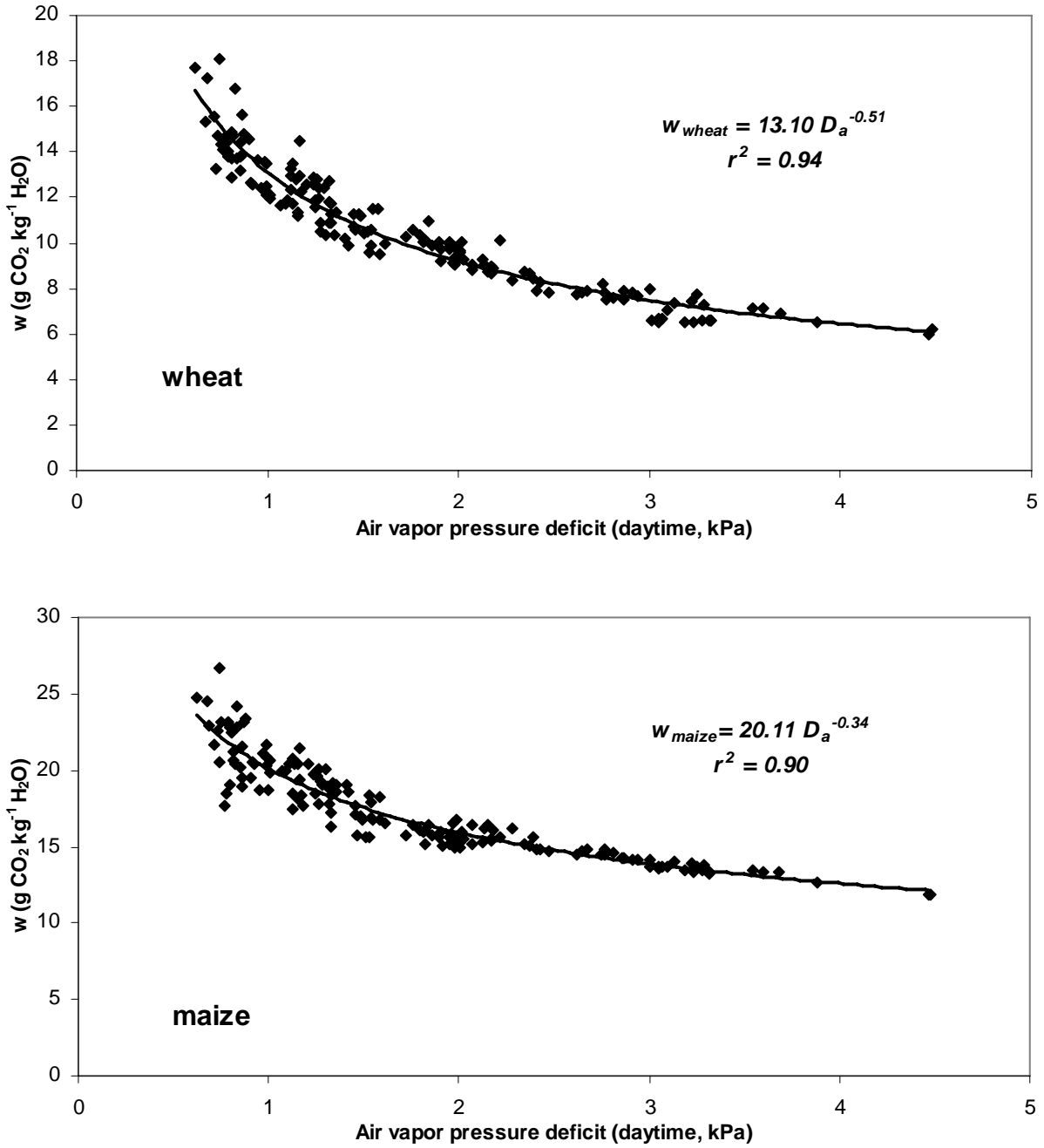
Figure 3. Transpiration use efficiency (B/T, g CO_2 kg^{-1} H_2O) as a function of the air water vapor pressure deficit (daytime, kPa) for wheat and maize.

$$w_{wheat} = 40.13\ ET_o^{-0.81}$$
$$r^2 = 0.89$$

$$w_{maize} = 39.22\ ET_o^{-0.49}$$
$$r^2 = 0.72$$
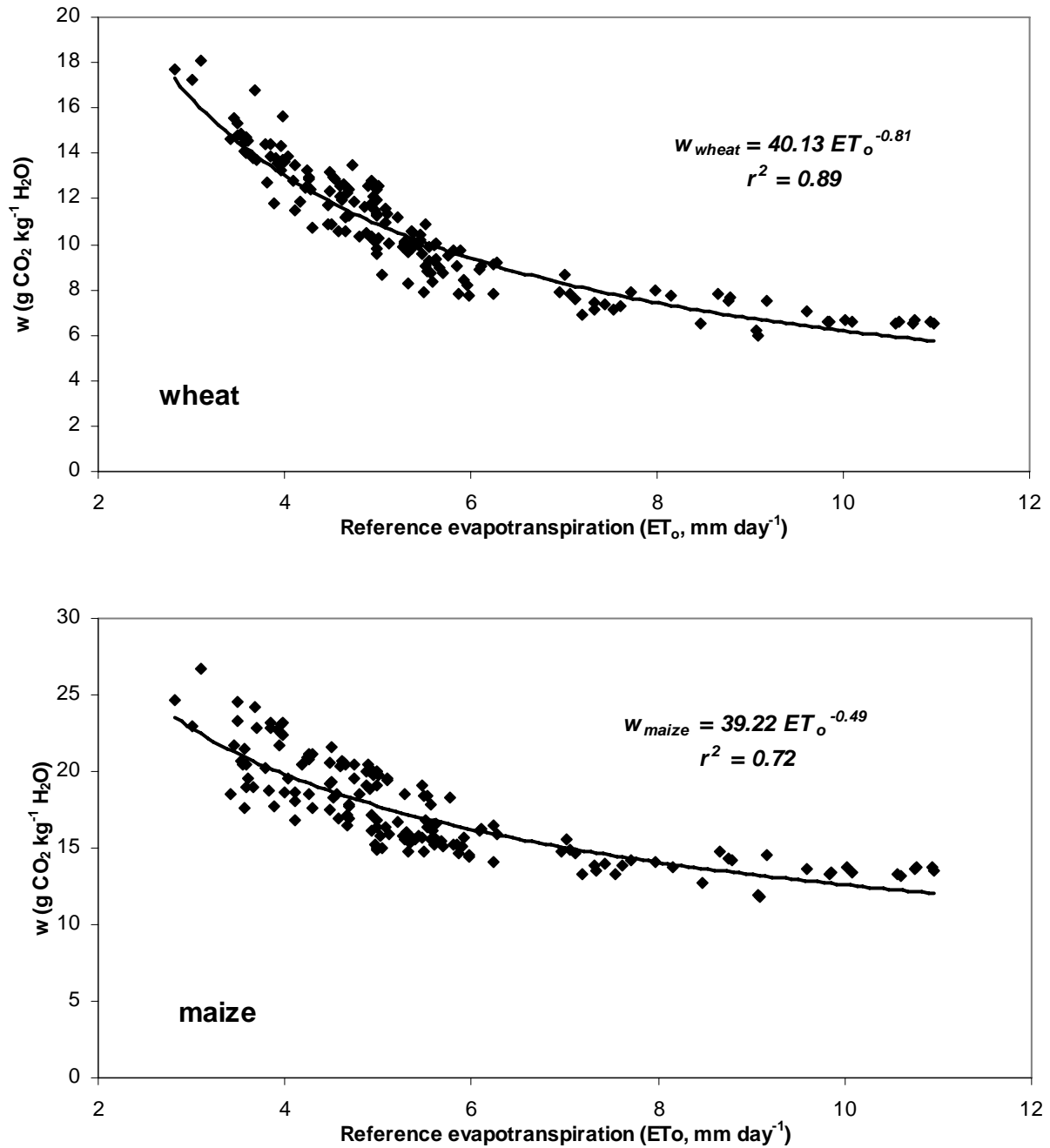
Figure 4. Transpiration use Efficiency (B/T, g CO_2 kg^{-1} H_2O) as a function of reference evapotranspiration (ET_o in mm day^{-1}) for wheat and maize.

Figure 5 reaffirms that the variability in Table 2 is not random, but can be explained to a large extent when k_{Da} values are plotted vs. D_a or ET_o. A linear equation was fitted to the k_{Da} values and included in the figure. It seems that D_a was able to explain k_{Da} variability better than ET_o, which presented a larger scattering, particularly for wheat. These results confirm that: 1) k_{Da} is not a constant value and, 2) k_{Da} increases when D_a and ET_o increases. The significant conclusion is that the use of Eq. (4) to estimate w has to considerer local calibration of k_{Da} to be transferable. The linear response obtained for k_{Da} should facilitate transferability through field calibration based on a few points across the environmental range. The fitted linear equations included in each figure, can be used as k_{Da} estimators for climatic conditions characterized by different D_a or ET_o.

Figure 5. Variability of k_{Da} (g CO_2 kg^{-1} H_2O kPa) as a function of the daytime vapor pressure deficit (D_a ; kPa), and the reference evapotranspiration (ET_o, mm day^{-1}) for wheat and maize.

In an attempt to explain k_{ETo} variability, k_{ETo} values were plotted vs. D_a and ET_o (Fig. 6). Fitted linear equations are included in the figure. Figure 6 shows that k_{ETo} variation in wheat does not correlate well with variations in climatic conditions represented by D_a or ET_o. However the relatively low CV and s determined that a mean value of 55.87 (g CO_2 m^{-2}) can be used as a constant regardless of the climatic environment, supporting the view of Steduto and Albrizio (2005). Nevertheless, some response of k_{ETo} for wheat when the ET_o gradient is increasing was observed (Fig. 6), suggesting some benefit of using the fitted equation in situations with high evaporative demand.

A different scenario was found in maize (see Table 2). Figure 6 shows that k_{ETo} (maize) did not correlate well with variations in D_a, and that the variability was better explained by ET_o, although ET_o alone was not able to account for the entire variability due to weather. It can be concluded that k_{ETo} is not a constant and, therefore, experimental values can not be transferred among locations with different climate. The linear equation presented here to estimate k_{ETo} as function of ET_o for maize should be taken as first approximation to overcome the transferability problem.

$k_{ETomaize} = 10.59\ D_a + 75.60$

$r^2 = 0.30$

$k_{ETowheat} = 0.68\ D_a + 54.66$

$r^2 = 0.01$

$k_{ETomaize} = 7.66\ ET_o + 51.86$

$r^2 = 0.71$

$k_{ETowheat} = 1.52\ ET_o + 47.44$
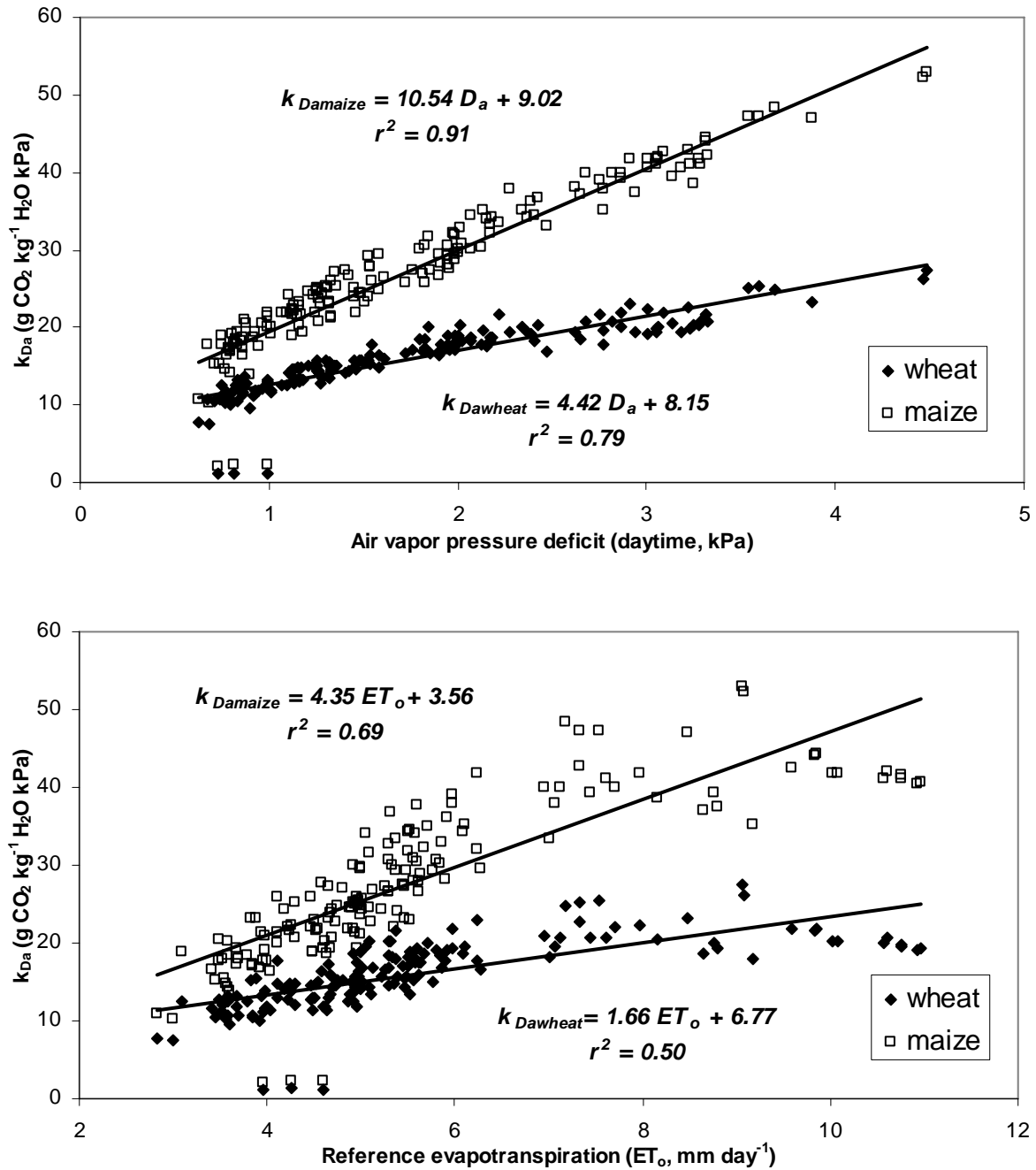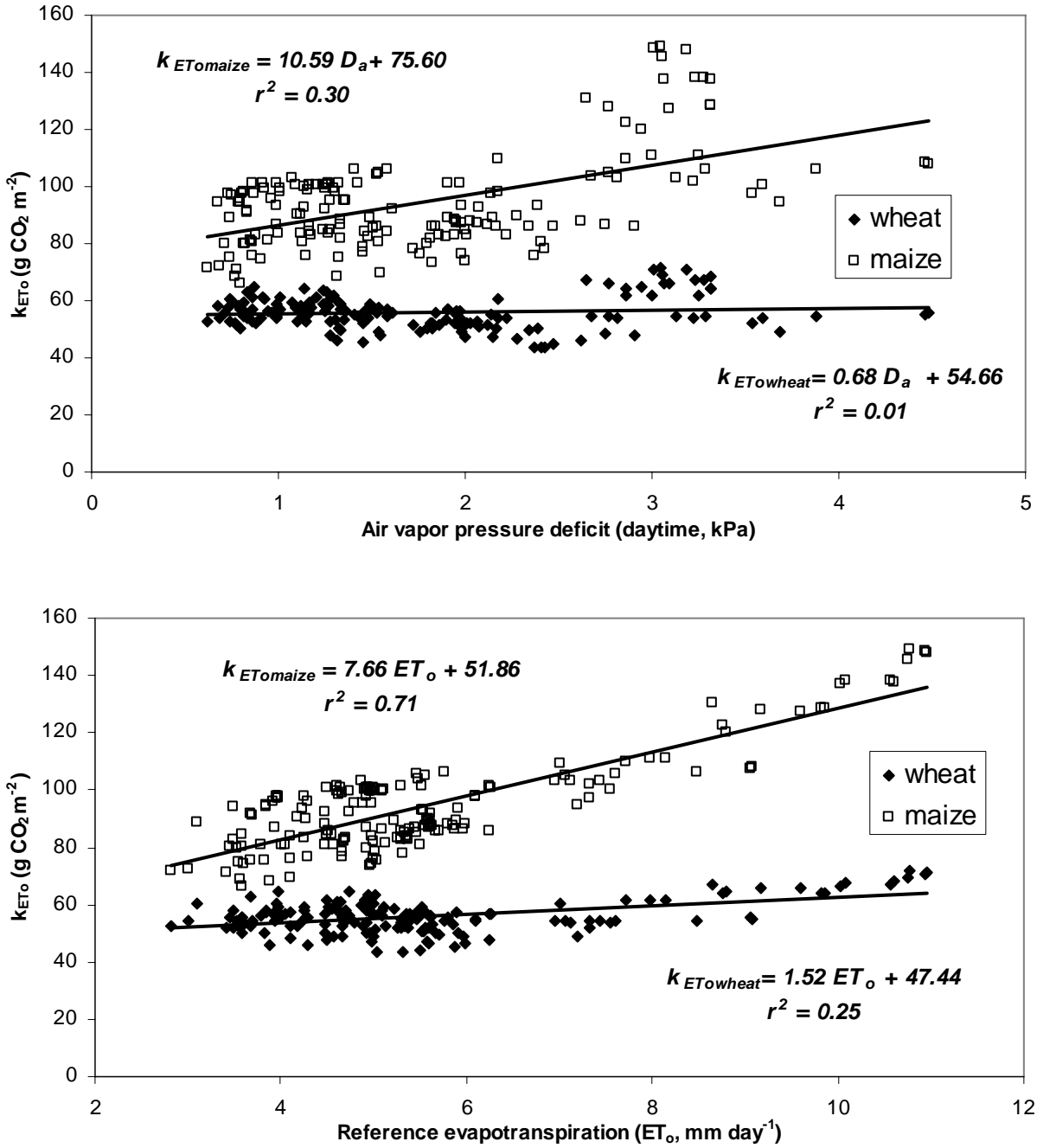
$r^2 = 0.25$

Figure 6. Variability of k_{ETo} (g CO_2 m^{-2}) as a function of the daytime vapor pressure

deficit (D_a ; kPa), and the reference evapotranspiration (ET_o, mm day^{-1}) for wheat and maize.

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4. CONCLUSIONS

The simulation results showed that w is not constant across climatic environments, so that values determined in one location can not be readily transferred to another. However, w as a function of D_a and ET_o was well described by a power function, with D_a explaining 94% and 90% of the w variability for wheat and maize, respectively, and ET_o explaining 89% and 72%, respectively. The dispersion around the fitted lines was lower with D_a and ET_o values greater than 2 kPa and 7 mm/day, respectively.

Normalization of the k_{Da} and k_{ETo} parameters by D_a and ET_o was not able to properly account for the effect of weather variability, resulting in parameters too variable to be readily transferred across locations for both wheat and maize.

It was found that the transferability of these parameters can be dramatically improved when they are plotted against D_a (in the case of k_{Da}) or ET_o (in the case of k_{ETo}), with linear functions describing well the relations and explaining 79% and 91% of k_{Da} variability for wheat and maize, and 71% of k_{ETo} variability for maize. The k_{ETo} for wheat correlated weakly with ET_o, explaining only 25% of its variability. However, the overall coefficient of variation of this parameter across eight locations was about 10%, so that the use of a constant k_{ETo} value is not unreasonably, although is not a perfect solution.

The simulation–based equations presented here are offered as a first approximation to overcome the spatial transferability of w, k_{Da} and k_{ETo}, but field validation will be required before adoption is recommended.

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CHAPTER THREE

Evaluation of Simulation-based Methods for Estimating Transpiration-Use Efficiency of Wheat and Maize

ABSTRACT

In the precedent chapter, equations were developed to estimate crop transpiration–use efficiency (w, g CO_2 kg^{-1} H_2O) and to determine parameters used in simple approaches to estimate w (k_{Da}, g CO_2 kg^{-1} H_2O kPa; k_{ETo}, g CO_2 m^{-2} ground area). These equations estimate w, k_{Da}, and k_{ETo} as a function of climatic conditions represented by daytime air vapor pressure deficit (D_a) or reference crop evapotranspiration (ET_o). To develop the equations, simulations using a mechanistic canopy transpiration and photosynthesis model were performed using weather data from eight world locations with contrasting climate. In this chapter, equations expressed in terms of CO_2 assimilation per unit ground area were converted to aboveground biomass per unit ground area using a conversion factor f_{abg} (0.36 for wheat, and 0.33 for maize), and evaluated with available field data. Experimental w data in the literature are not only scarce, but they are variable due to differences in cultivars, crop management, methods to estimate crop transpiration and biomass, and other sources of variability. Despite these limitations, the simulation–based equations to estimate w and k_{Da} of wheat and maize, and k_{ETo} of maize appeared to be good estimators of observed values, while k_{ETo} of wheat was better represented by a single value across climatic conditions.

1. INTRODUCTION

Crop transpiration–use efficiency (w), defined as the ratio of biomass (B) produced per unit of water transpired (T), has been used to evaluate crop productivity as a function of water supply. A few approaches have been proposed to estimate w as a function of climatic conditions. Two of these approaches will be considered here:

$$w = \frac{k_{Da}}{D_a} ; \quad \text{(Bierhuizen and Slatyer, 1965; Tanner and Sinclair, 1983)} \qquad (1)$$

$$w = \frac{k_{ETo}}{ET_o} ; \quad \text{(Steduto and Albrizio, 2005)} \qquad (2)$$

where k_{Da} and k_{ETo} are crop–dependent parameters, D_a is the daytime air vapor pressure deficit and ET_o is the reference crop evapotranspiration (Allen et al., 1998). It is commonly accepted that both k_{Da} and k_{ETo} are reasonably conservative so that values determined experimentally in one location can be readily transferred to another (Ehlers and Goss, 2003) while D_a and ET_o (Eqs. (1) and (2), respectively) will account for the effect of climatic differences on w. Equations 1 and 2 have been used and accepted as reasonable predictors of w (eg. Stöckle et al., 1994; Sinclair and Seligman, 1995; Steduto and Albrizio, 2005). However, concerns about the transferability of k_{Da} have been raised recently (Kemanian et al., 2005), while Steduto and Albrizio (2005) have claimed that k_{ETo} is a more stable and transferable parameter than k_{Da}.

During the development of the companion chapters (Chapters 1 and 2), the transferability of k_{Da} and k_{ETo} was tested for well developed and non stressed crops using a mechanistic canopy transpiration and photosynthesis model (CTP). The model was applied using data from eight world locations to determine k_{Da} (g CO_2 kg^{-1}H_2O kPa) and k_{ETo} (g CO_2 m^{-2} ground area) values

for wheat and maize. The results of this analysis indicated that these parameters were not stable, but tended to increase along climatic gradients represented by increasing D_a (kPa) or ET_o (mm day^{-1}). In chapter 2, equations were proposed to estimate w, k_{Da} and k_{ETo} as a function of D_a or ET_o. These equations, obtained by computer simulation, will require field verification before they can be used.

The CTP model calculates w as mass of CO_2 assimilation per mass of water transpired, which cannot be compared directly with literature data usually expressed as aboveground biomass produced per mass of water transpired. To transform CO_2 assimilation to aboveground biomass production, Monteith (1981) suggested that: 1) the biomass produced by a crop can be assumed a constant fraction of CO_2 assimilation, and 2) the fraction of CO_2 assimilation loss by respiration (f_r) is often 0.35 to 0.45. Therefore, as a first approximation, the following factor times CO_2 assimilation would estimate biomass production:

$$f_{DM} = 0.682(1 - f_r) \tag{3}$$

where 0.682 is the ratio of molecular weights of CH_2O and CO_2. To estimate aboveground biomass, the fraction of biomass apportioned to the roots has to be discounted. Thus, the conversion factor of mass of CO_2 fixation to aboveground biomass is given by:

$$f_{abg} = \frac{0.682(1 - f_r)}{(1 + r)} \tag{4}$$

where r is the root to shoot fraction. Considering a r value for wheat and maize of 0.20 to 0.30 (Lorenz and Lal, 2005), f_{abg} should range between 0.29 and 0.37. Using w field data available in literature (Table 1 and 2) and w from the simulation-based equations (Chapter 2), f_{abg} was optimized and determined to be 0.36 and 0.33 for wheat and maize, respectively. Thus, the

equations from chapter 2 to estimate w (g kg^{-1}), k_{Da} (Pa) and k_{ETo} (g m^{-2}), expressed in terms of aboveground biomass are:

$$w_{wheat} = 4.65\, D_a^{-0.51} \tag{5}$$

$$w_{maize} = 6.77\, D_a^{-0.34}$$

$$k_{Dawheat} = 1.57 D_a + 2.89 \tag{6}$$

$$k_{Damaize} = 3.54 D_a + 3.04 \tag{7}$$

$$k_{ETowheat} = 0.54 ET_o + 16.82 \tag{8}$$

$$k_{ETomaize} = 2.58 ET_o + 17.45 \tag{9}$$

The main objective of this work was to evaluate the validity of these equations to estimate w, k_{Da} and k_{ETo} across climatic conditions through comparison with field data.

2. MATERIALS AND METHODS

Experimental data suitable for the calculation of w, k_{Da}, and k_{ETo} were obtained from published articles and direct communication with selected researchers. In a few instances, experimental values for these parameters were readily available, but in most cases they were derived from raw data. The quality of the available data differed and was classified as follows: a) complete data set available including daily crop transpiration, crop above ground biomass accumulation, and daily measurements of global solar radiation (MJ m^{-2} s^{-1}), air temperature (°C), air relative humidity and wind speed; b) daily crop transpiration was not reported; c) data set includes daily crop evapotranspiration instead of transpiration, and d) crop transpiration and biomass are presented as total for the period, and D_a and ET_o are averaged for the same period. For type (a) no additional effort was needed and k_{Da} and k_{ETo} were estimated as the slope of the linear regression between biomass accumulation and the daily integration of the quotient transpiration to daytime D_a (eg. Tanner, 1981; Condon et al., 1993; Kemanian et al., 2005) or the daily integration of the quotient transpiration to ET_o (e.g. Steduto and Albrizio, 2005). For type (b), daily crop transpiration was simulated using the CTP model, and k_{Da} and k_{ETo} were estimated with the regression method explained in (a). For type (c), crop transpiration was computed as: $T = ET(1 - \tau_{bt})$, where T is crop transpiration, ET is the measured evapotranspiration and τ_{bt} is the estimated fraction of incident beam irradiance that penetrates the canopy and reaches the soil surface. The k_{Da} and k_{ETo} were computed with the regression method. For type (d), k_{Da} and k_{ETo} were reported or estimated as the product of w times D_a or

ET_o. Transpiration–use efficiency in all the cases was estimated as the quotient between total aboveground biomass and transpiration for the period tested.

Daytime D_a was computed as 2/3 of the maximum D_a for each day (e.g. Kemanian et al., 2005), determined from maximum temperature and minimum relative humidity. Daily ET_o calculations were carried out daily as proposed by Allen et al. (1998).

Tables 1, 2, 3 and 4 summarize the available data and their quality type.

Table 1. Wheat transpiration use efficiency (w) and k_{Da} as reported or calculated from data obtained in literature. Q refers to the quality of the data as described in the text.

Source	Site	Q	variety	w (g kg^{-1})	k_{Da}(Pa)	D_a (kPa)	observations
(1)	Mederrin, Australia	d	Gutha	4.61	4.43	0.96	1987
			Gameny	4.49	4.67	0.96	
			Purple Straw	3.95	4.11	0.96	
(2)		d	Timgalen	5.00	4.08	0.82	1973,D1,preanthesis
				4.30	5.10	1.19	1973,D1,postanthesis
				4.90	4.50	0.92	1973,D2,preanthesis
				3.90	4.80	1.23	1973,D2,postanthesis
				3.60	3.87	1.07	1973,D3,preanthesis
				3.10	4.20	1.35	1973,D3,postanthesis
				4.20	3.81	0.91	1975,D1,preanthesis
				4.10	4.80	1.17	1975,D1,postanthesis
				3.40	3.33	0.98	1975,D2,preanthesis
				3.40	4.73	1.39	1975,D2,postanthesis
(3)	Werribee, Australia	d	Bank	6.60	4.74	0.7	1984
				7.53	4.82	0.64	1985
			Quarrion	7.24	4.93	0.68	1984
				8.61	5.26	0.61	1985
(4)	Moombooldool,	a	Gutha	7.10	3.80	0.54	1985, preanthesis

	Australia						
			Quarrion	5.87	4.79	0.71	
(5)	Toowoomba, Australia	d	Hattog	3.93	4.58	1.18	1993
(6)	Nottinghamshire, UK	d	Soissons	5.29	3.44	0.6	1994
				5.77	3.75	0.63	1995
			Maris Huntsman	6.20	4.03	0.60	1994
				6.22	4.04	0.63	1995
(7)	Pullman, WA	a	WB926R	4.59	5.90	1.13	Pooling 1998/1999
(8)	Bushland, TX	c		5.10	5.30	1.21	1989/90
				3.94	4.63	1.01	1991/93 NE Lysimeter
				3.59	4.32	0.95	1991/92 SE Lysimeter
				3.94	4.00	1.04	1992/93 NW Lysimeter
				4.38	4.55	1.02	1992/93 SW Lysimeter
(9)	Aleppo, Syria	b	Cham1	4.45	5.53	1.32	1990
			Huarina	4.64	6.00	1.32	1990
(10)	Pucawan, Australia	d	Average of	6.20	3.43	0.51	preanthesis, low N
			Cometz,	5.20	2.70	0.51	preanthesis, high N
			Janz and	3.74	5.83	1.54	postanthesis, low N
			Kulin	3.39	5.22	1.54	postanthesis, high N

(1) Siddique et al. (1990); (2) Doyle and Fischer (1979); (3) Connor et al. (1992); (4) Condon et al. (1993); (5) Meinke et al. (1977); (6) Foulkes et al. (2001); (7) Marcos (2000); (8) Howard, T. (personal communication) (9) Pala et al. (1996); (10) Angus and van Herwaarden (2001).

Table 2. Maize transpiration use efficiency (w) and k_{Da} as reported or calculated from data obtained in literature. Q refers to the quality of the data as described in the text.

Source	Site	Q	variety	w (g kg^{-1})	k_{Da} (Pa)	D_a (kPa)	observations
(1)	Logan, UT	d	Utahybrid 544a and NKPX–20	4.12	8.4	2.04	1974/1975
	Ft. Collins, CO	d	NKPX–20 and Pioneer 3955	4.88	10.2	2.09	1974/1975
	Davis, CA	d	Funks 4444	4.93	9.9	2.01	1974/1975
(2)	Elora, ontario	d	PAG SXIII	6.12	6.06	0.99	1981– low density
				8.25	8.16	0.99	1981–high density
				6.64	6.93	1.04	1982–high N
				7.44	7.55	1.02	1982–low N
(3)	Davis, CA	c		5.14	9.92	2.04	1974
(4)	Prosser, WA	b		6.01	9.90	1.68	2004 –early seeding
				6.3	8.85	1.6	2004 –late seeding
(5)	Bushland, TX	c	Pioneer 3124	6.56	8.58	1.42	1990 NE Lysimeter
			Pioneer 3245	5.69	8.81	1.7	1990 SE Lysimeter
			Pioneer 3245	5.21	6.88	1.38	1994 NW Lysimeter
(6)	Lebanon , Bekaa valley	d	Manuel	4.18	13.83	3.31	1998

(1) Ehlers and Goss (2003), extracted from Tanner and Sinclair (1983); (2) Walker (1986); (3) Acevedo (1975); (4) Kremer (2004, not published); (5) Howard, T. (personal communication); (6) Karam et al. (2003).

Table 3. Wheat transpiration use efficiency (w) and k_{ETo} as reported or calculated from data obtained in literature. Q refers to the quality of the data as described in the text.

Source	Site	Q	variety	w (g kg^{-1})	k_{ETo} (g m^{-2})	ET_o (mm day^{-1})	observations
(1)	Bushland, TX	c		5.10	26.86	5.35	1989/90
				3.94	19.17	4.27	1991/93 NE Lysimeter
				3.59	16.66	3.87	1991/92 SE Lysimeter
				3.94	19.14	4.76	1992/93 NW Lysimeter
				4.38	21.57	4.72	1992/93 SW Lysimeter
(2)	Aleppo, Syria	b	Cham1	4.45	16.67	3.80	1990
			Huarina	4.64	18.50	4.01	1990

(1) Howard, T. (personal communication); (2) Pala et al. (1996).

Table 4. Maize transpiration use efficiency (w) and k_{ETo} as reported or calculated from data obtained in literature. Q refers to the quality of the data as described in the text.

Source	Site	Q	variety	w (g kg^{-1})	k_{ETo} (g kg^{-1})	ET_o (mm day^{-1})	observations
(1)	Davis, CA	c		5.14	29.5	5.84	1974
(2)	Prosser, WA	b		6.01	32.36	5.41	2004 –early seeding
				6.3	28.32	4.50	2004 –late seeding
(3)[bc]	Bushland, TX	c	Pioneer 3124	6.56	35.46	5.62	1990 NE Lysimeter
			Pioneer 3245	5.69	35.53	6.62	1990 SE Lysimeter
			Pioneer 3245	5.21	28.80	5.52	1994 SE Lysimeter
(4)	Lebanon , Bekaa valley	d	Manuel	4.18	57.54	13.04	1998

(1) Acevedo (1975); (2) Kremer (2004, not published); (3) Howard, T. (personal communication) (4) Karam et al. (2003).

2.1 Evaluation of the simulation-based equations

Qualitative evaluation of the performance of the simulation–based equations to estimate w and k_{Da} as a function of D_a, and k_{ETo} as a function of ET_o, was performed through graphical inspection, considering the trend of the observed (Tables 1, 2, 3, and 4) and simulation-based values.

The use of the simulation–based equations for actual field applications was tested by comparing their estimations with that of similar equations developed from observed data. The comparative analysis was performed by sampling from field and simulation-based equations at fixed intervals along a climatic gradient represented by D_a or ET_o within a range typical for commercial growth of wheat or maize and where most of the observed data were collected. The comparison was quantified as follows:

$$\overline{D}_e = 100 \, n^{-1} \sum_{1}^{n} \left(\frac{abs(S_i - F_i)}{S_i} \right) \tag{10}$$

where $\overline{D}_e$ is the average relative difference of estimation (percent), S_i is the w, k_{Da} or k_{ETo} values estimated with simulation–based equations, F_i is the w, k_{Da} or k_{ETo} values estimated with the observation–based equations, and n is the number of pair of data. A low $\overline{D}_e$ implies that the mean difference along the weather gradient of parameters estimated with the observation– and simulation–based equations is low, and vice versa.

3. RESULTS AND DISCUSSION

Simulated and observed data points of transpiration–use efficiency, plotted as a function of daytime D_a , are shown in Fig. 1. The scattering of the simulated points is an indication of other climatic sources of variability that remain unexplained. Overall, the simulated and observed values present a similar trend, but with larger scattering of the latter. The scattering of observed data is enhanced by differences in varieties, crop management; methods to estimate crop transpiration, biomass sampling method, other sources of experimental error, and methods of calculation (see data quality). Simulated w, k_{Da} and k_{ETo} data included a wide range of climatic conditions while observed values were concentrated in the common range suitable for commercial growth of wheat or maize. The comparative analysis was limited to the observed range of climatic variability. In the case of wheat, the observed w data are concentrated in the 0.5 to 1.6 kPa D_a range, with a 60% of the data from environments with D_a lower than 1kPa. Maize is grown in a wider range of conditions (1 to 3.3 kPa). Figure 2 shows power functions fitted to the observed and simulated w values as function of D_a. These equations are similar, particularly in the case of wheat. For wheat the index $\overline{D}_e$ had value of 4.8%, and a maximum value (n=1) of 9.2% at 1.6 kPa, whereas for maize a mean value of 6.5% and a maximum value (n=1) of 12.3% at 3.3 kPa was found. It can be concluded that the variability of w with D_a is supported by observed and simulated data, and that the simulation–based equations can be used as a tool to transfer w across climatic conditions beyond that covered by available field data.
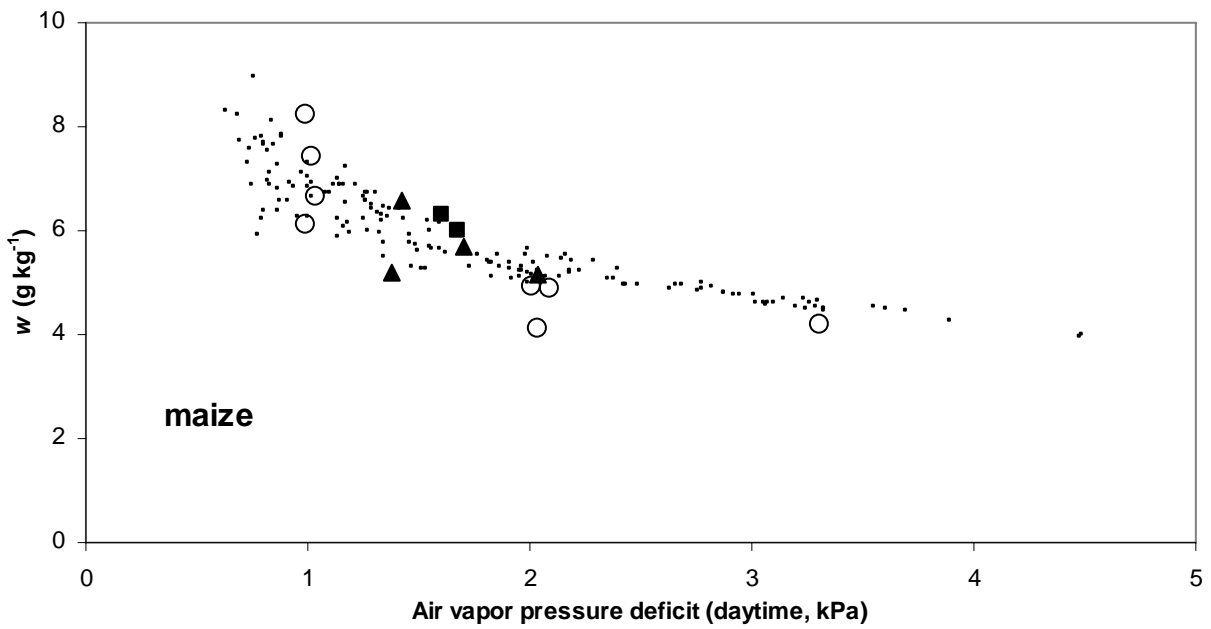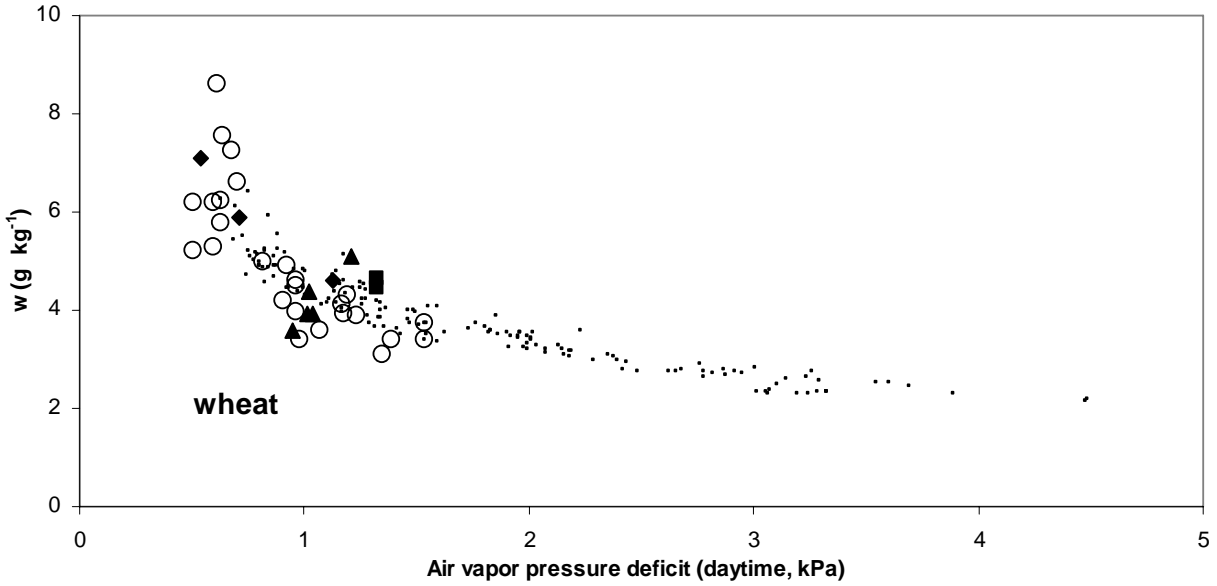
Figure 1. Transpiration use efficiency (w, g biomass k g^{-1} H$_2$O) as a function of the air water

vapor pressure deficit (daytime, kPa) for wheat and maize. -: simulated outputs; ♦: type (a) data;

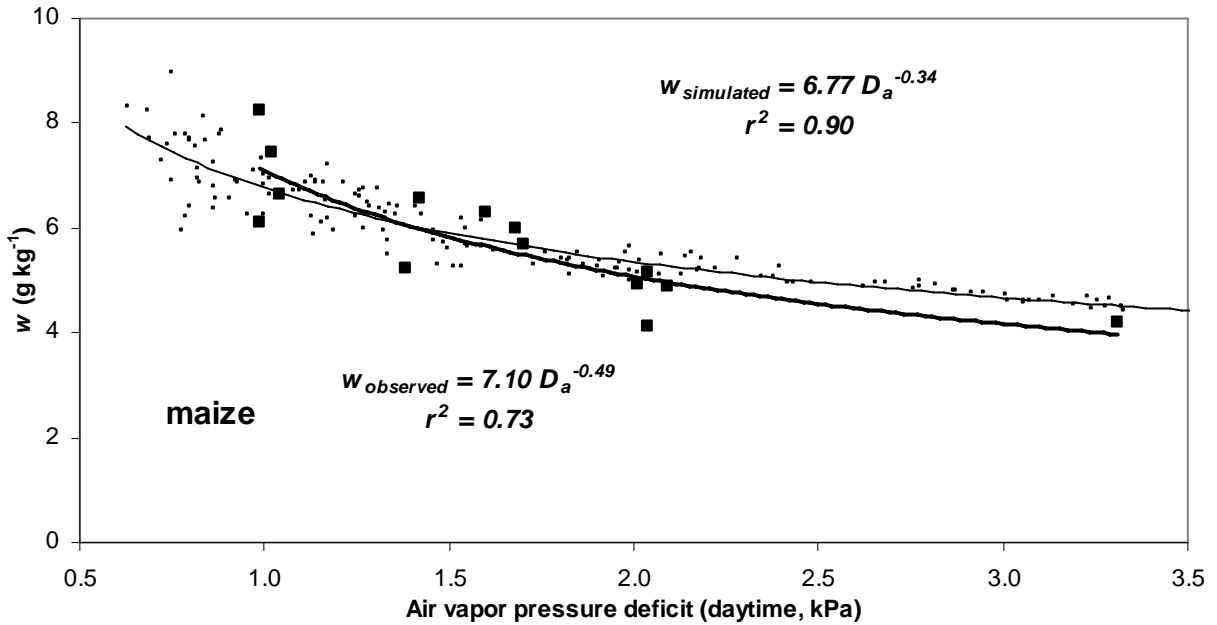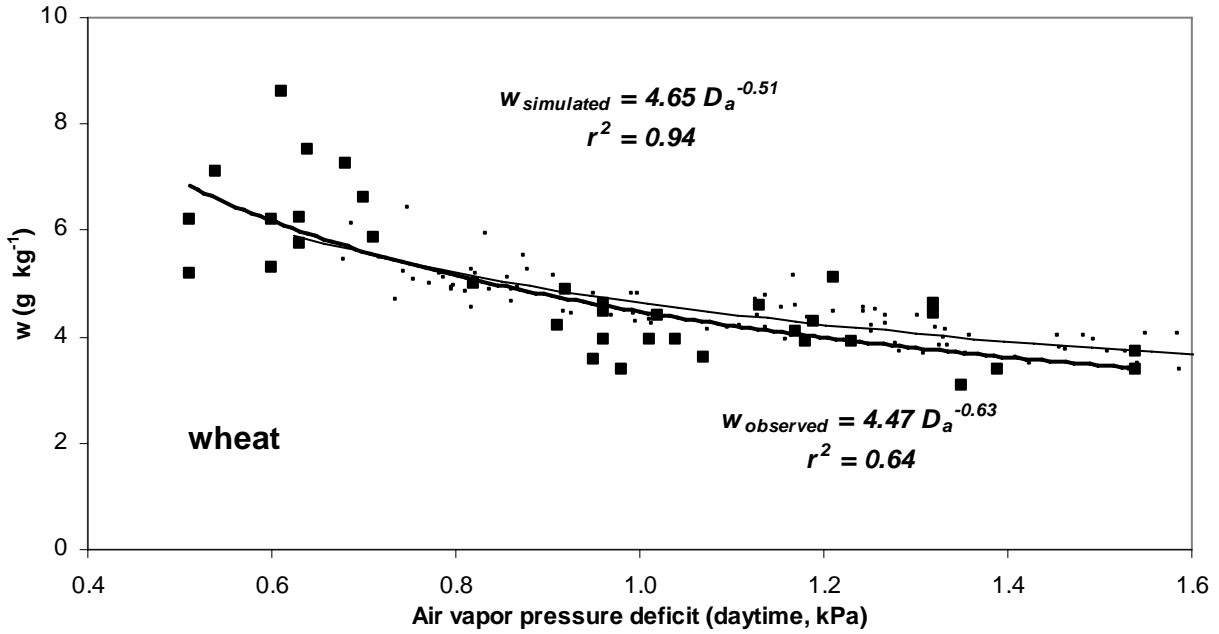■ : type (b) data; ▲: type (c) data;○: type (d) data.

Figure 2. Variability *w* as a function of the vapor pressure deficit (daytime; kPa) for wheat and maize. +: simulated data; ▪: observed data; — : fitted line for simulated data; ▬: fitted line for observed data.

Figure 3 presents observed and simulated values of k_{Da}, showing a good visual agreement between the two sets of values. Figure 4 includes linear regressions of observed and simulated k_{Da} values as a function of D_a. Again, the comparative analysis was limited to the range of climatic variability of the observed data. The equations are very similar, in fact remarkably similar in the case of wheat. For wheat the index $\overline{D}_e$ had a value of 2.5% and a maximum value ($n=1$) of 3.8% at 0.5 kPa , whereas for maize had a value of 4.8% and maximum value ($n=1$) of 8.9% at 3.3 kPa. These results indicate that: a) k_{Da} is not a constant across a climatic gradient, b) the variation of k_{Da} with D_a is supported by simulated and observed data, c) the simulated linear equations , which includes a wider range of climatic conditions, can be used as tool to extrapolate experimentally–determined k_{Da} values or to select k_{Da} values for estimation of w and crop productivity, and d) the use of the CTP model as a means to determining k_{Da} values for crops other than wheat and maize appears promising and would constitute a valuable tool, particularly considering that data is limited or non existent for most crops.
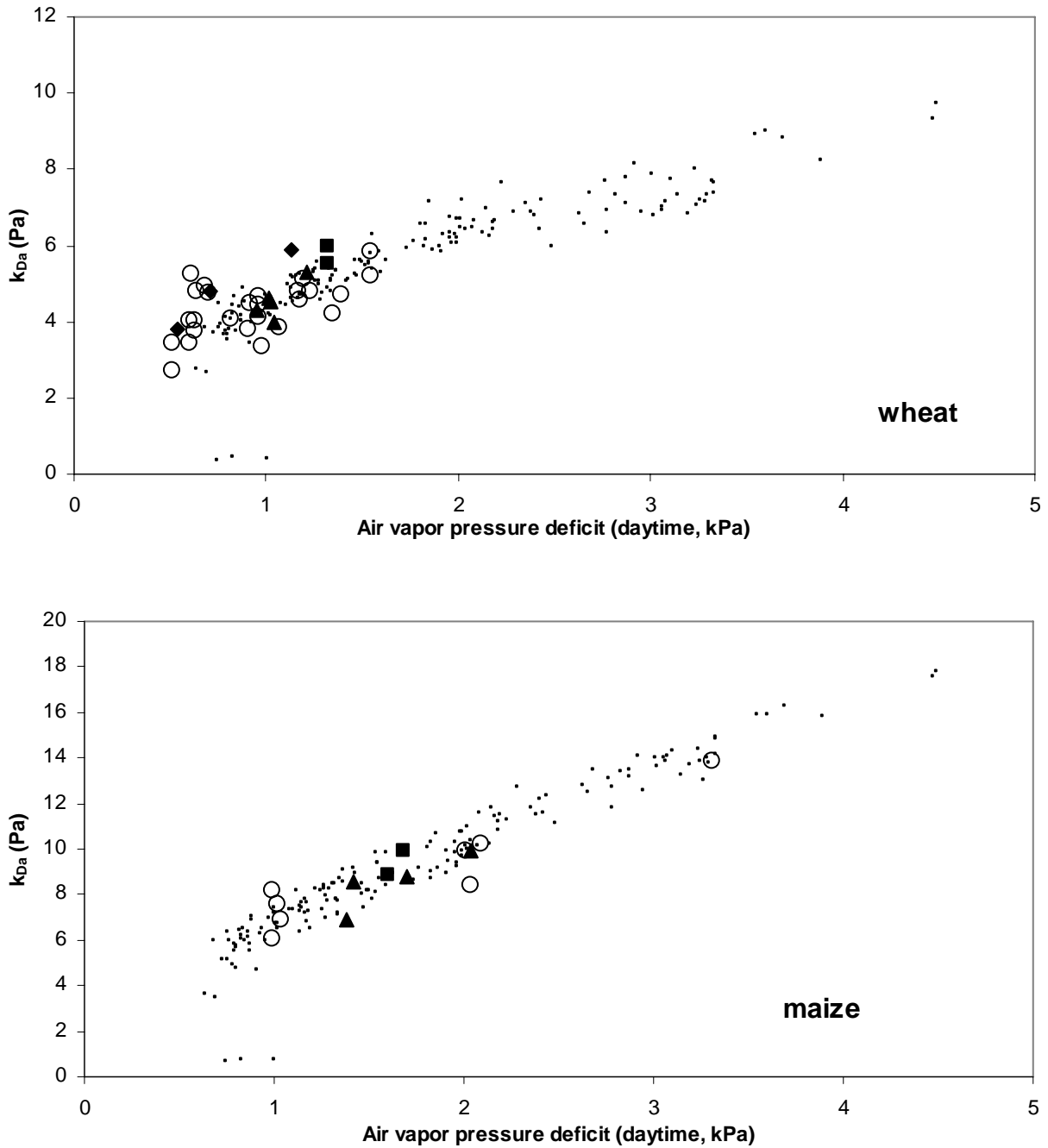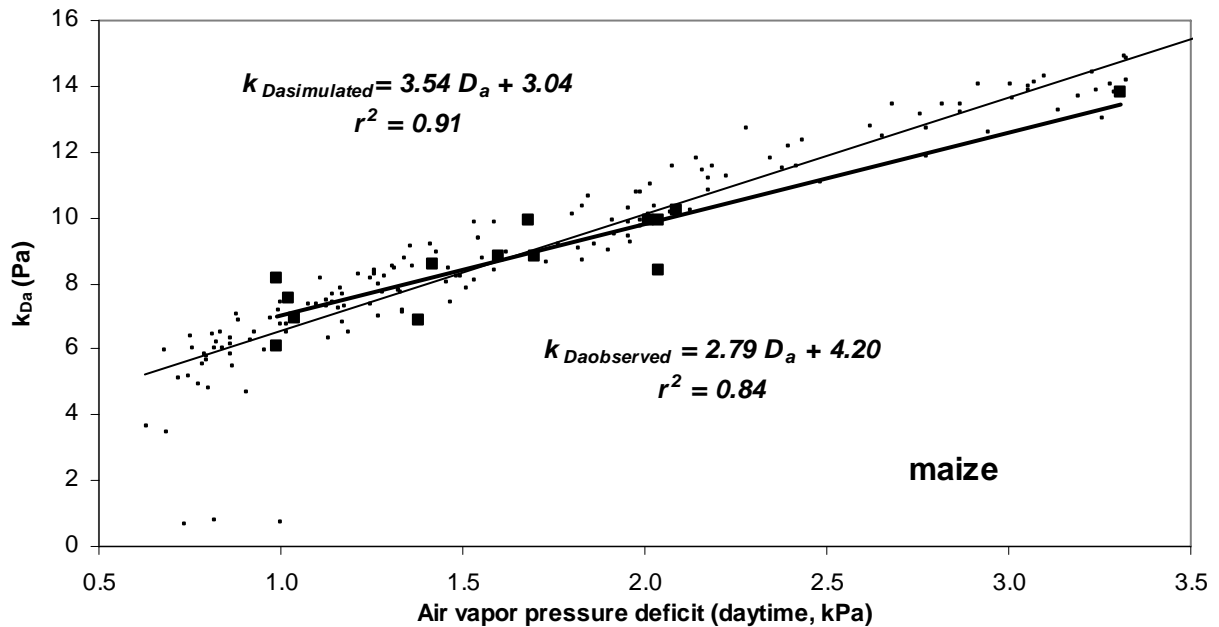
Figure 3. Variability of k_{Da} (Pa) as a function of the vapor pressure deficit (daytime; kPa) for wheat and maize. -: simulated data; ♦: type (a) data; ■ : type (b) data; ▲: type (c) data; ○: type (d) data.
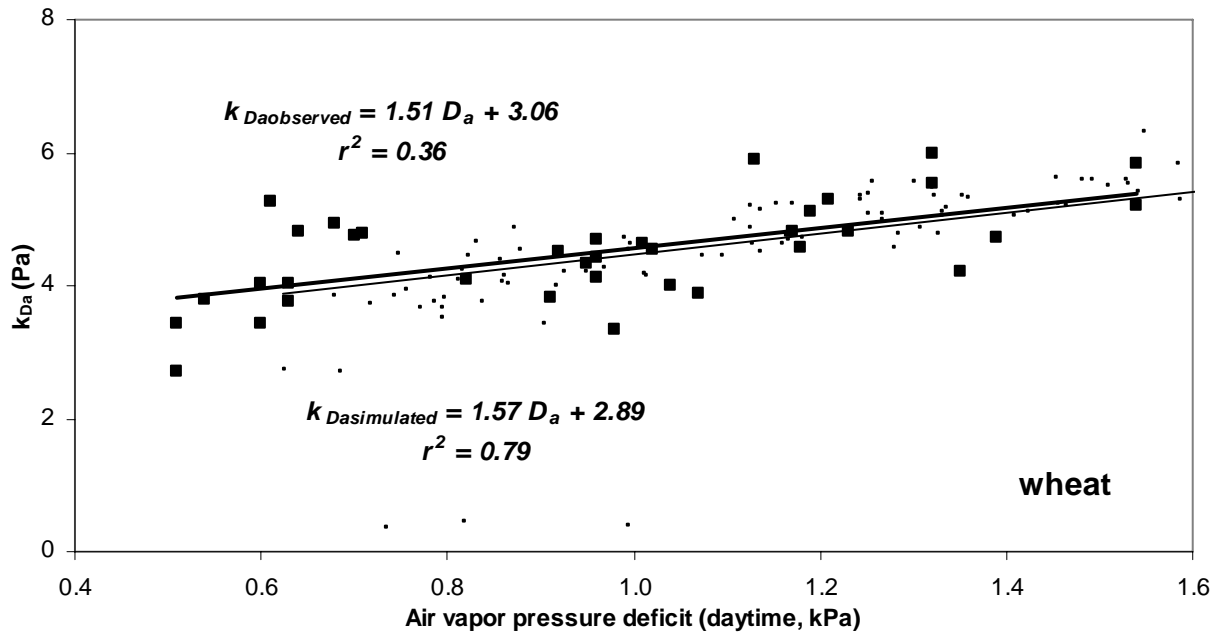
Figure 4. Variability of k_{Da} (Pa) as a function of the vapor pressure deficit (daytime; kPa) for wheat and maize. -: simulated data; ■: observed data; — : fitted line for simulated data; ▬: fitted line for observed data.

Figure 5 shows observed and simulated values of k_{ETo}. In chapter 2 it was concluded that, in the case of wheat, an average k_{ETo} value could be used as a constant regardless of climatic differences. This appears to be the case in the ET_o range where the observed values are gathered (3.8 to 5.4 mm day^{-1}), although Fig. 5 suggests that a linear regression (not shown) of simulated k_{ETo} as a function of ET_o could provide a better approximation than the average value under conditions of unusually high ET_o. There is a fair agreement between observed and simulated values within the ET_o range of the observed data with and average k_{ETo} of 19.79 and 19.81 g m^{-2} for observed and simulated data respectively, but the low number of observed data makes it difficult to be more conclusive. In the case of maize, the available observed data was also scarce, but its ET_o range was wider (4.5 to 13 mm day^{-1}), allowing a better comparison. A good visual agreement of simulated and observed k_{ETo} is noticeable. Dispersion of observed data for maize followed the same trend that the simulated data. Figure 6 shows linear regressions of observed and simulated k_{ETo} values for maize as function of ET_o. The simulated and observed linear equations are similar. The index $\overline{D}_e$ had a value of 6.4 % and a maximum value (n=1) of 12.3% at 13.04 mm day^{-1}. It can be concluded that, in the case of maize, the variation of w with ET_o is supported with observed and simulated data, and that the simulation–based equation can be used as a tool to transfer experimentally–determined values to other locations.
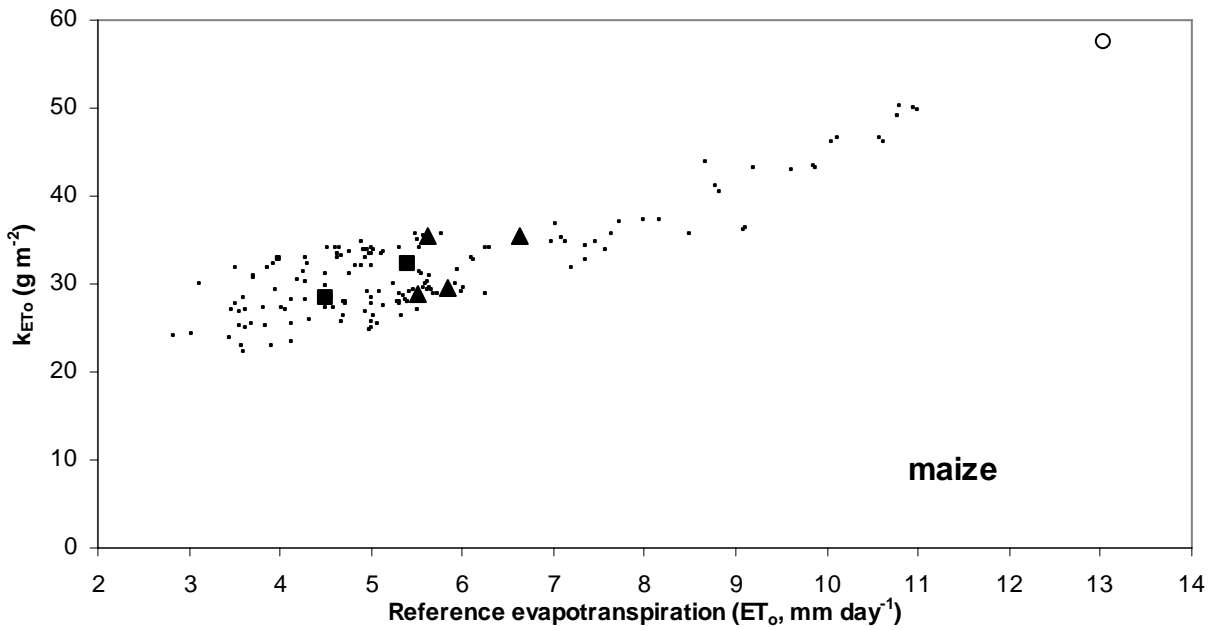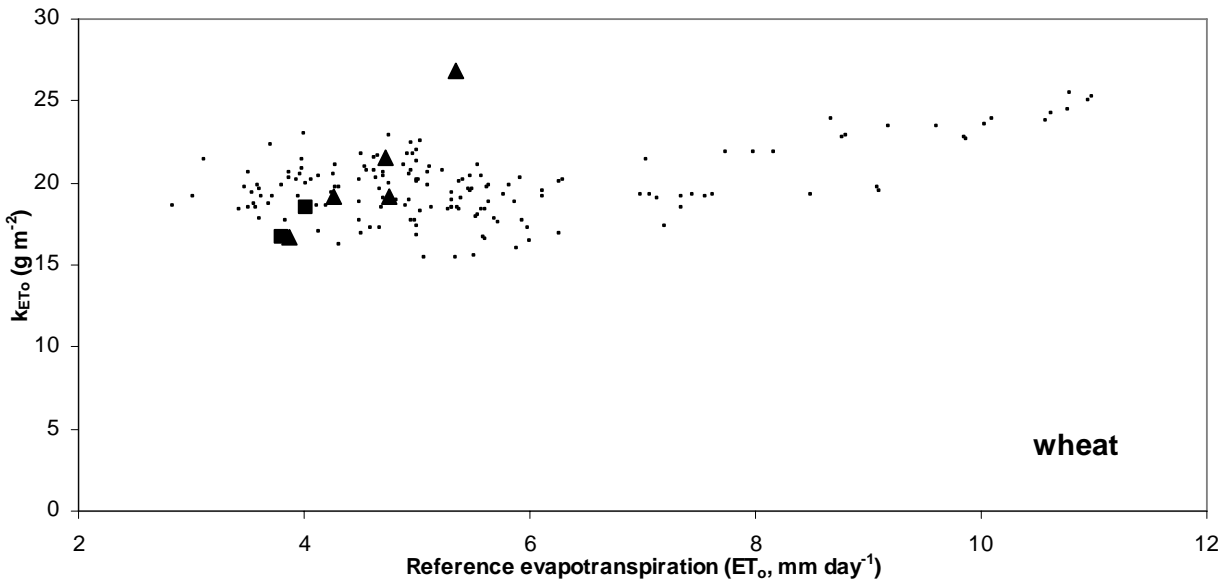
Figure 5. Variability of k_{ETo} (g m^{-2}) as a function of the reference evapotranspiration (ET_o; mm day^{-1}) for wheat and maize. -: simulated data; ■ : type (b) data; ▲: type (c) data; ○: type (d) data.
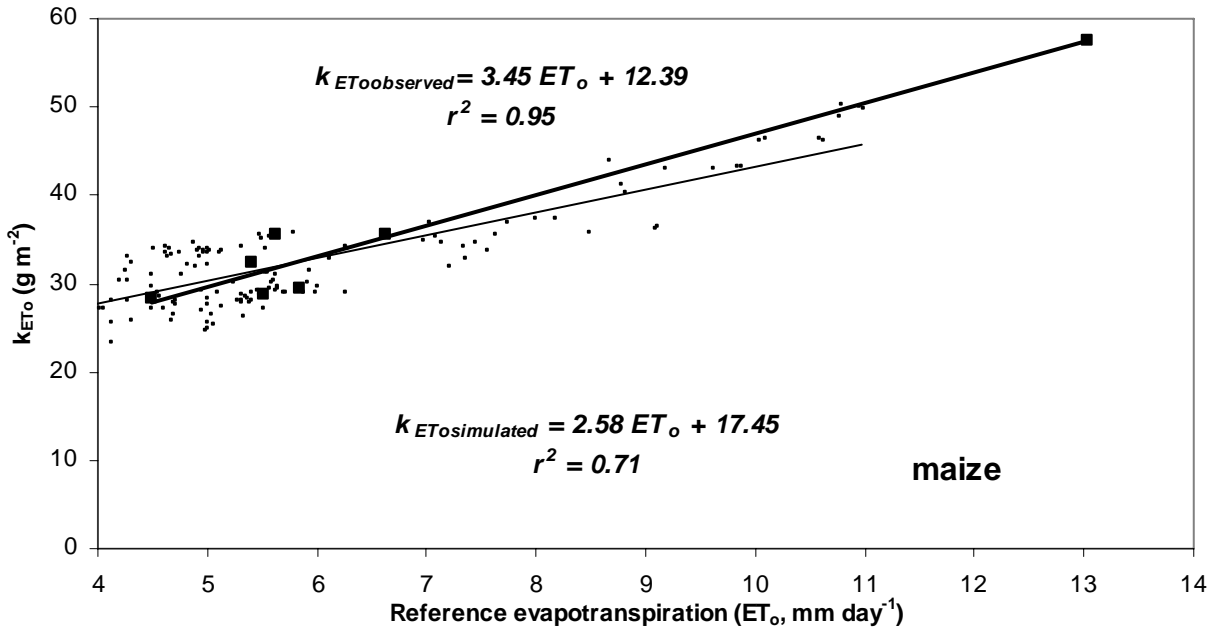
Figure 6. Variability of k_{ETo} (mm day^{-1}) as a function of the reference evapotranspiration (ET_o) for maize. -: simulated outputs; ■: observed data; — : fitted line for simulated data; ▬: fitted line for observed data.

4. CONCLUSIONS

The validity of the simulation–based equations to estimate w and k_{Da} as functions of D_a, and k_{ETo} as a function of ET_o was demonstrated using observed data from different sources.

The simulation–based power equations to estimate w as function of D_a for wheat and maize showed to be reliable estimators, with the variation of w with D_a being supported by both observed and simulated data.

The simulation–based linear equations to estimate k_{Da} as a function of D_a showed to be robust estimators of the observed values for wheat and maize, with D_a able to explain most of the variation of k_{Da} across a wide climatic range. Their use to extrapolate experimentally–determined k_{Da} values or to select k_{Da} values for estimation of w and crop productivity is supported by these results.

The performance of the functions to estimate k_{ETo} could not be tested with sufficient data, however some comments can be made. In the case of wheat, the use of an average k_{ETo} value appears as a reasonable approximation to estimate w. In contrast, k_{ETo} for maize appeared correlated with variations of ET_o.

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APPENDIX

Appendix A. Hourly environmental variables

The curve which represent the temperature and relative humidity daily pattern was derived by "fitting two terms of a Fourier series to the average of many days of hourly data that had been normalized so that the minimum was zero at the maximum was 1" (Campbell and Norman, 1998). The result is a dimensionless diurnal function ($\Gamma(t)$):

$$\Gamma(t) = 0.44 - 0.46\sin\left(\frac{\pi t}{12} + 0.9\right) + 0.11\sin\left(\frac{2\pi t}{12} + 0.9\right) \tag{A.1}$$

where t is the time of day in hours. By this function, the temperature ($T(t)$(°C)) for any time of the day is given by:

$$T(t) = T_x^{i-1}\Gamma(t) + T_n^i\left[1 - \Gamma(t)\right] \qquad 0 < t \le 5 \tag{A.2}$$

$$T(t) = T_x^i\Gamma(t) + T_n^i\left[1 - \Gamma(t)\right] \qquad 5 < t \le 14 \tag{A.3}$$

$$T(t) = T_x^i\Gamma(t) + T_n^{i+1}\left[1 - \Gamma(t)\right] \qquad 14 < t < 24 \tag{A.4}$$

and the relative humidity ($HR(t)$) for any time of the day is given by:

$$HR(t) = HR_n^{i-1}\Gamma(t) + HR_x^i\left[1 - \Gamma(t)\right] \qquad 0 < t \le 5 \tag{A.5}$$

$$HR(t) = HR_n^i\Gamma(t) + HR_x^{i+1}\left[1 - \Gamma(t)\right] \qquad 5 < t \le 14 \tag{A.6}$$

$$HR(t) = HR_n^i\Gamma(t) + HR_x^i\left[1 - \Gamma(t)\right] \qquad 14 < t < 24 \tag{A.7}$$

where, T_x and HR_x are the daily maximum temperature and relative humidity, respectively; and T_n and HR_n are the minimum daily temperature and relative humidity, respectively. The superscript, i represent the present day, $i-1$ is the previous day, and $i+1$ is the next day.

After that, the hourly air water vapor pressure deficit (D_a, kPa) is computed through:

$$D_a(t) = e_s(t)\left(1 - \frac{HR(t)}{100}\right) \tag{A.8}$$

where $e_s(t)$ is the hourly water vapor pressure at saturation given by:

$$e_s(t) = 0.611\exp\left(\frac{17.502T(t)}{T(t) + 240.97}\right) \tag{A.9}$$