Actual Evapotranspiration for Sugarcane Based on Bowen Ratio-Energy Balance and Soil Water Balance Models with Optimized Crop Coefficients

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Abstract
Evapotranspiration is an important parameter to evaluate soil water deficit and water use efficiency, especially in locations with irregularly distributed precipitation. The aim of this study was to assess the daily actual evapotranspiration (ETa) estimated by the Thornthwaite and Mather soil water balance adapted for crops (ThM) and by the dual Kc method with the crop coefficients optimized from inverse modeling and by the adjustment suggested in the FAO-56 bulletin. The models were optimized and evaluated with actual evapotranspiration determined by the Bowen ratio – energy balance method (ETβ) for sugarcane at full canopy closure grown in Alagoas state, northeastern Brazil. The objective function of the inverse problem was defined in terms of ETβ and ETa estimated by the ThM or dual Kc method by optimizing the single crop coefficient (Kc) and the basal crop coefficient Kcb, respectively. Optimized Kc (1.05) and Kcb (1.03) were lower than those adjusted by the Kc FAO56 method (Kc = 1.25 or Kcb = 1.20), with optimized Kc slightly higher than the Kc obtained experimentally (1.01 ± 0.08). ETa estimated by the ThM and dual Kc method with optimized crop coefficients had similar high precision (r2 > 0.79) and accuracy (dm > 0.93 and RMSE < 0.30 mm d⁻¹). However, using the coefficients adjusted from the FAO56 method overestimated ETa in both models.

Keywords Thornthwaite and Mather · Dual Kc · Inverse modeling
1 Introduction

Evapotranspiration (evaporation + transpiration) are the main components of the global water cycle, and advances in the measurement and modeling of these fluxes from different fields are required to ultimately model the global hydrological cycle and evaluate its effects on the global climate (Godoy et al. 2021). At more regional and local scales, evaporation is the main variable of the water balance of lakes and basins, especially in arid and semiarid regions (Ashrafzadeh et al. 2019; Biazar et al. 2020). Evapotranspiration (ET) is a keystone variable for watershed management and is essential for irrigation design and scheduling to mitigate crop yield reduction due to soil water deficits or drought (Cammalleri et al. 2013; Dingre and Gorantiwar 2020; Tigkas et al. 2020; Marin et al. 2020). Therefore, ET is a main input variable in soil water and crop models that can be used to evaluate crop water use efficiency, growth and yield (Angaleeswari and Ravikumar 2019).

Sugarcane is one of the main cultivated crops in the world and is best known for its production of sugar and ethanol and, more recently, as a source of energy (Dingre and Gorantiwar 2020; Marin et al. 2020; Matos et al. 2020). As it is an annual crop, it experiences soil water deficits in many regions due to irregularly distributed precipitation, leading to reduction in evapotranspiration and thus in crop yield. This can be even more relevant in locations where the dry season coincides with the summer, such as in northeastern Brazil, or in semi-arid regions (Lyra et al. 2010; Cammalleri et al. 2013; Rocha et al. 2018; Dingre and Gorantiwar 2020). Therefore, estimation of sugarcane ET in such locations is essential to assess crop yield responses to soil water deficit and to support the irrigation design and scheduling (Dingre and Gorantiwar 2020).

ET can be determined by several methods, generally grouped according to the related physical principles and measurement scales (Rana and Katerji 2000). Micrometeorological methods, such as the Bowen ratio – energy balance (BREB) and the eddy covariance method, are suitable to determine ET for large fields on flat surfaces with sufficient fetch and for time scales ranging from 15 to 60 min (Liu and Xu 2018; Rocha et al. 2018). The BREB method stands out in terms of its physical simplicity and the required instrumentation and has been used in several applications, such as in the determination of crop coefficients and evaluation of ET models (Inman-Bamber and McGlinchey 2003; Margonis et al. 2018; Marin et al. 2020). However, due to its simplifications and assumptions (Perez et al. 1999), the BREB does not always lead to physically consistent results, which must be evaluated to filter inconsistent values. In this regard, the simple and physically based approach proposed by Perez et al. (1999) has been frequently used.

For agricultural applications such as irrigation and water user efficiency evaluations, the actual ET (ETa) can be estimated through soil water balance (SWB) models (Mattar et al. 2016). Several SWB models are described in the literature, varying from the simple tipping bucket approach considering only one soil layer — Thornthwaite and Mather (1955) and WOFOST model (van Diepen et al. 1989), two layers — dual Kc method (Allen et al. 1998) and, or multiple layers — AquaCrop model (Steduto et al. 2012) to physically based models based on the Richards equation — SWAP (Kroes et al. 2017) and HYDRUS model (Simunek et al. 2009). In general, the greater the number of layers and coefficients, the greater the difficulty of applying these models due, for example, to data collection limitations, instability and uncertainty propagation. The use of more complex physically based models requires more understanding of the involved processes and information about soil hydraulic parameters and boundary conditions, which are not always available (van den Berg et al. 2002; Angaleeswari and Ravikumar 2019).
Thornthwaite and Mather’s SWB has a simple procedure to estimate $ET_a$, often applied at regional (e.g., climate classification) or watershed scales and ten-day or monthly time intervals. The method originally required only the total available water (TAW, the so-called available water capacity), total precipitation, and potential evapotranspiration (Thornthwaite and Mather 1955). However, applying this method for crops needs to take into account other parameters, such as the crop coefficient ($K_c$) and effective root system depth (Lyra et al. 2010). Alternatively, ET can be estimated by separating $K_c$ into two parts: i) an evaporation coefficient ($K_e$) and ii) a coefficient related to plant transpiration ($K_{cb}$) by using the dual $K_c$ method as detailed in the FAO-56 bulletin (Allen et al. 1998; Cammalleri et al. 2013). Parameters such as $K_c$ and $K_{cb}$ are available in FAO-56 for several crops or groups of crops for each growth stage, as well as an equation to adjust these parameters to local climate conditions (Allen et al. 1998). However, some authors have found different $K_c$ values from those obtained by the adjusting equations, leading to inaccurate $ET_a$ estimates (Cammalleri et al. 2013; Mattar et al. 2016). Therefore, in some cases, these values need to be determined experimentally to attain more accurate estimates (Dingre and Gorantiwar 2020; Marin et al. 2020). Alternatively, $K_c$ or $K_{cb}$ can be obtained by inverse modeling techniques, allowing optimization of input model parameters based on model simulations and a smaller number of observed data (Moura Neto and da Silva Neto 2013; Cammalleri et al. 2013, Mattar et al. 2016). It can be even more important for determining $K_{cb}$, whose direct determination relies on the plant transpiration measurement, which is more challenging. Inverse procedures for parameter estimation have been widely used in many disciplines, for instance, in soil water flow problems to infer parameters for soil hydraulic functions and root water uptake models (Hupet et al. 2003; Santos et al. 2017b; Angaleeswari and Ravikumar 2019). However, few attempts have been made to derive crop coefficient parameters through this technique or similar approaches (Zhang et al. 2011; Cammalleri et al. 2013), especially with simple tipping bucket models to estimate ET.

The aim of this study was to assess the performance of Thornthwaite and Mather’s SWB adapted for crops (hereafter referred to as ThM) and the dual $K_c$ method in estimating daily actual evapotranspiration with crop coefficients obtained by inverse modeling. These models were also assessed with crop coefficients derived from the adjustment suggested in the FAO-56 bulletin. The model comparison and optimization were performed with actual evapotranspiration determined by the Bowen ratio – energy balance method ($ET_\beta$) for sugarcane at full canopy closure grown in Alagoas state, northeastern Brazil.

2 Materials and Methods

2.1 Study Area, Crop Treatments and Micrometeorological Measures

An experiment was carried out at the Campus of Engineering and Agricultural Sciences of the Federal University of Alagoas, Rio Largo region, Coastal Tablelands of Alagoas State, northeastern Brazil (09°28’02” S; 35°49’43” W; 127 m). According to the Thornthwaite classification, the region has a humid, megathermal climate with moderate water deficit in the summer and excess of water in the winter. The average annual rainfall is 1,818 mm, concentrated in the period between April and August. The air temperature ranges from 19.3 (August) to 31.7 °C (January), with an annual average of 25.4 °C. The soil is a Yellow Oxisol, with the following physical properties: soil water contents at field capacity
and permanent wilting point equal to 0.207 m$^3$ m$^{-3}$ and 0.124 m$^3$ m$^{-3}$, respectively; soil density of 1468 kg m$^{-3}$; and total porosity of 0.423 m$^3$ m$^{-3}$ (Lyra et al. 2010).

The micrometeorological measurements were performed in a plantation of sugarcane (Saccharum ssp.) cv. RB92579 in the plant cycle under rainfed conditions. The crop was planted on 09/16/05 and harvested on 11/12/06, totaling a cycle of 440 days. Details about the main environmental and agronomical characteristics can be found in Santos et al. (2017a).

A micrometeorological tower installed inside the plantation was used as a basis for the sensors measuring the net radiation components and the atmospheric property profiles (air temperature and humidity). The area had a fetch of approximately 150 m in the predominant wind direction, and it was surrounded by commercial sugarcane plantations. Net radiation was measured with a net radiometer (CNR1 model, Kipp & Zonen, Netherlands) and kept at 0.5 m above the crop canopy. Air temperature and relative humidity were measured by two thermohygrometers (HMP35 model, Vaisala, Finland) installed at 0.2 and 2.2 m above the canopy. The soil heat flux was measured by a heat flux plate (HFT3, Campbell Scientific Inc., USA) at a depth of 0.08 m. All measurements were performed every 10 s and averaged every 10 min by a datalogger (CR10X, Campbell Scientific Inc., USA). In the BREG method, we used the hourly averages of the measured micrometeorological variables.

The meteorological variables (global solar radiation, maximum and minimum air temperatures, rainfall, wind speed and air humidity) used as input in the ThM and dual Kc method were measured with an automated agrometeorological station (CR10X, Campbell Sci., Logan, Utah).

### 2.2 Bowen Ratio–Energy Balance

The Bowen ratio – energy balance (BREB) is based on the energy conservation law, which, when applied to the soil–plant-atmosphere system, can be expressed by the simplified energy balance approach:

$$ R_n - G - H - LE = 0, \tag{1} $$

where $R_n$ is the net radiation ($W$ m$^{-2}$), $G$ is the soil heat flux ($W$ m$^{-2}$), $H$ is the sensible heat flux ($W$ m$^{-2}$), and LE is the latent heat flux ($W$ m$^{-2}$).

The Bowen ratio ($\beta$) is defined as the ratio between the $H$ and the $LE$ at the surface following the hypothesis of equality between eddy diffusivity coefficients for heat and water vapor ($K_h = K_w$) (Bowen 1926; Margonis et al. 2018), that is:

$$ \beta = \frac{H}{LE} \cong \gamma \left( \frac{\Delta T}{\Delta e} \right), \tag{2} $$

where $\gamma = (c_p \ P_{\text{atm}})/(0.622 \ \lambda)$ is the psychrometric coefficient (kPa °C$^{-1}$), $c_p$ is the specific heat of the air at constant temperature (1004.8 J kg$^{-1}$ °C$^{-1}$), $P_{\text{atm}}$ is the atmospheric pressure (101.23 kPa), $\lambda$ is the latent heat of vaporization ($2.45 \times 10^6$ J kg$^{-1}$), and $\Delta T$ and $\Delta e$ are the difference in air temperature (°C) and actual air vapor pressure (kPa), respectively, between the two heights above the canopy.

Inserting Eq. (2) into Eq. (1) results in the following expressions for LE and H:
where \( R_n \) and \( G \) are measured directly in the field.

The conventions used for energy flux signs were \( R_n \) positive downward, \( G \) positive from the surface downward and \( LE \) and \( H \) positive upward (opposite to the gradient direction). The variations \( \Delta T \) and \( \Delta e \) were obtained by the difference between the lower and upper measurement heights. The Bowen ratio and fluxes were estimated on an hourly time step.

The hourly ET from the BREB was obtained by dividing the \( LE \) by \( \lambda \) and multiplying by 3600 s, and the daily actual ET (\( ET_a \)) was obtained by integration throughout the day.

BREB components were evaluated between 07/03/06 and 07/27/06, which coincided with part of the region’s rainy season. This period was chosen because the crop was at full canopy closure and the rainfall observed was sufficient to maintain the soil water content close to field capacity.

### 2.3 Data Selection Criteria for the BREB

We used the physically based approach proposed by Perez et al. (1999) to assess the BREB consistency. In this approach, first \( LE \) and \( H \) estimates must be consistent with the gradient upward and downward flux conventions. By rearranging Eqs. (2), (3) and (4), and based on the convention adopted for the fluxes and the calculation of \( \Delta e \) and \( \Delta T \), Perez et al. (1999) found:

\[
\frac{\Delta e}{LE} = \gamma \frac{\Delta T}{H} = \frac{\Delta e(1 + \beta)}{R_n - G} < 0, \tag{5}
\]

According to Eq. (5), the validity of the BREB depends on a series of combinations of \( (R_n - G) \), \( \Delta e \) and \( \beta \) signs around \(-1\) satisfying the inequality. Perez et al. (1999) provide a summary of all the combinations leading to physically consistent values of the method that we adopted to select the set of consistent data.

When \( \beta \to -1 \), the BREB also leads to inconsistent flux values, since \( LE \) and \( H \) tend to infinity. Therefore, it is necessary to define an interval for \( \beta \) around \(-1\), that is, \(-1 - |\varepsilon| < \beta < -1 + |\varepsilon|\), at which the fluxes are physically inconsistent and need to be discarded. Perez et al. (1999) suggested this interval to be dependent on the \( \beta \) accuracy estimation, and by applying error analysis in Eq. (2) they found that \( \varepsilon = \delta \beta \) is given by:

\[
\varepsilon = \frac{\delta \Delta e + \gamma \delta \Delta T}{\Delta e}, \tag{6}
\]

where \( \delta \Delta e \) and \( \delta \Delta T \) are the precision of the sensors measuring the water vapor pressure (0.03 kPa) and air temperature (0.2 °C) gradients, respectively.

The procedures above make it possible to obtain physically consistent flux values by the BREB. However, as the BREB is an indirect method, it is also necessary to assess the accuracy of the flux values. The uncertainties in LE estimation by the BREB can be evaluated by determining the relative error of LE (Perez et al. 1999). Thus, by applying the error analysis in Eq. (3) it follows that:
where $\delta R_n$ and $\delta G$ are the accuracies of the $R_n$ and $G$ measurements, respectively.

### 2.4 Soil Water Balance - Thornthwaite and Mather (Single $K_c$)

The Thornthwaite and Mather sequential water balance (ThM) adapted for crops (Lyra et al. 2010) requires daily crop evapotranspiration ($ET_c$, mm d$^{-1}$) values, which were determined by the single crop coefficient ($K_c$) method presented in FAO-56:

$$ET_c = ET_o K_c,$$

where $ET_o$ is the daily reference evapotranspiration ($ET_o$, mm d$^{-1}$) and $K_c$ is the crop coefficient. The $ET_o$ was estimated by the parameterized Penman–Monteith method described in the FAO-56 bulletin ($ET_o$-FAO56) (Allen et al. 1998).

To determine the $K_c$ during the growing period, a cycle of 440 days was divided into the initial stage (length of 60 days), crop development stage (124 days), mid-season stage (196 days) and late season stage (60 days). The adjusted initial (1.15), crop development (1.25) and late season (0.75) $K_c$ values were used to interpolate the $K_c$ curve over the entire growing season (Lyra et al. 2010). The initial $K_c$ ($K_{c,ini}$) was adjusted following the approach presented in FAO56, whereas the mid-season ($K_{c,miq}$) and late season ($K_{c,end}$) crop coefficients were adjusted as follows (Allen et al. 1998):

$$K_c = K_{c(tab)} + [0.04(u_2 - 2) - 0.004(RH_{min} - 45)](\frac{h}{3})^{0.3},$$

where $K_{c(tab)}$ is a tabulated $K_c$ given in FAO-56, $RH_{min}$ (%) is the daily minimum relative humidity, and $h$ (m) is the crop height for the mid-season (2.4 m) or late season (2.8 m) stage, measured in the field.

Estimating actual evapotranspiration ($ET_a$, mm d$^{-1}$) requires the computation of daily SWB, which was obtained by the Thornthwaite and Mather (1955) method, expressed in a generic way as:

$$\Delta SW = (SW_i - SW_{i-1}) = (P_i + I_i) - ET_{a,i} - S_i,$$

where $\Delta SW$ is the available soil water rate (SW, mm d$^{-1}$); $P$ is the precipitation rate (mm d$^{-1}$); I is the irrigation rate (mm d$^{-1}$), which was disregarded in this work as the sugarcane was grown under rainfed conditions; and S is the water surplus rate (mm d$^{-1}$). The subscript terms i and i-1 represent the current and the previous day, respectively. Both $ET_{a,i}$ and $S_i$ in Eq. (10) are unknowns; thus, the equation is solved by the following procedure:

if $(P_i + I_i) - ET_{c,i} < 0$, $SW_i$, then

$$APWL_i = APWL_{i-1} - (P_i + I_i - ET_{c,i}),$$

$$SW_i = TAW_i \ exp(APWL_i/TAW_i),$$

else if $(P_i + I_i) - ET_{c,i} \geq 0$,

$$SW_i = SW_{i-1} + (P_i + I_i - ET_{c,i}),$$
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where APWL (mm d\(^{-1}\)) is the accumulated potential water loss and TAW (mm) is the total available soil water. When \((P_i + I_i) - ET_{ci} < 0\), \(S_i = 0\), and \(ET_{a,i}\) is determined by Eq. (10); otherwise (as by definition), \(ET_{a,i}\) equals \(ET_{ci}\), and \(S_i\) is obtained by Eq. (10). The APWL is calculated as a running sum of \((P + I)ET_c\) values during days when \((P + I)ET_c\) is negative (Eq. 11).

When applying the ThM model to a crop, the TAW (mm) is considered to vary with the effective root system depth \(z_r\) (m) as follows:

\[
TAW = 1000(\theta_{fc} - \theta_{wp})z_r,
\]

where \(\theta_{fc}\) and \(\theta_{wp}\) are the soil water contents at field capacity and permanent wilting point, respectively, and \(z_r\) was estimated for the entire growing period by the method proposed in Allen et al. (1998):

\[
z_{r,i} = [(K_{c,i} - K_{c,ini})/(K_{c,mid} - K_{c,ini})](z_{r,x} - z_{r,n}) + z_{r,n},
\]

where \(K_{c,i}\) is the crop coefficient of day \(i\), \(K_{c,ini}\) and \(K_{c,mid}\) are the initial and mid-season crop coefficients, respectively, and \(z_{r,n}\) (0.1 m) and \(z_{r,x}\) (0.3 m) are the minimum and maximum root system depths, respectively. At the intermediate and final stages, \(z_{r}\) was assumed to be constant and equal to \(z_{r,x}\).

2.5 Dual \(K_c\) - FAO-56

The dual \(K_c\) method, as described in the FAO-56 bulletin, also requires the \(ET_0\) estimate, which was also obtained by the \(ET_0\)-FAO56. Then, \(ET_0\) is estimated by Eq. (8) (Allen et al. 1998), but with \(K_c = K_{cb} + K_c\), where \(K_{cb}\) is the so-called basal crop coefficient and \(K_c\) is the soil evaporation coefficient. Differently from the single \(K_c\) method, the dual \(K_c\) method can estimate the \(ET_a\ [= ET_0 K_c]\), which is performed by separating the crop coefficient into two parts:

\[
K_c = K_s K_{cb} + K_e,
\]

where \(K_s\) is a water stress coefficient due to the soil water deficit, obtained as follows (Allen et al. 1998; Cammalleri et al. 2013):

\[
K_s,i = \frac{TAW - D_{r,i}}{TAW - RAW} = \frac{TAW - D_{r,i}}{(1 - p)TAW},
\]

where \(p (=0.45)\) is the maximum allowed depletion, corresponding to the TAW fraction that can be depleted from the root zone before drought stress conditions, \(RAW [= p TAW]\) is the readily available soil water (mm), and \(D_{r,i}\) is the soil water depletion at the root system depth (mm) at day \(i\). For \(D_r \leq RAW, K_s = 1\). The \(p\) value was tabulated in the FAO56 bulletin for sugarcane and based on soil texture.

Similar to the single crop coefficient method, the FAO-56 bulletin provides tabulated values for \(K_{cb,mid}\) (1.20) or \(K_{cb,end}\) (0.70). These values were adjusted with Eq. (9) by replacing \(K_c\) with the tabulated \(K_{cb}\). By setting \(K_{cb,ini}\) equal to 0.15, the \(K_{cb}\) curve throughout the cycle was interpolated similarly to that of \(K_c\), considering the same growing stage length presented previously.

\(K_c\) is given by the following equation:
where $K_r$ is a dimensionless soil evaporation reduction coefficient, $K_{c,x}$ is a value representing the daily upper limit of evaporation and transpiration from a vegetated surface, and $f_{ew}$ is the fraction of wetted soil exposed to radiation, given by:

$$f_{ew,i} = \min \left(1 - f_{c,i}f_w\right),$$

where $f_w (=1.0)$ is the average soil surface fraction wetted by rainfall or irrigation and $f_c$ is the average soil surface fraction covered by vegetation, which in the absence of measurements can be estimated by:

$$f_{c,i} = \max \left[\left(\frac{K_{c,b,i} - K_{c,n}}{K_{c,x} - K_{c,n}}\right)^{\left(1+0.5h_{i}\right)} , 0.01\right],$$

where $K_{c,b}$ is the basal crop coefficient at a particular day $i$ or period, $K_{c,n}$ is the minimum $K_c$ for dry bare soil, considered here as $K_{c,b,ini}$ (Allen et al. 1998), and $K_{c,x}$ was determined by the following equation:

$$K_{c,x,i} = \max \left[1.2 + \left[0.04\left(u_2 - 2\right) - 0.004\left(RH_{min} - 45\right)\right] \left(\frac{h_{i}}{3}\right)^{0.3}, (K_{cb,i} + 0.05)\right],$$

where $h$ (m) is the crop height at a particular growth stage.

In the FAO-56 bulletin, soil water evaporation is assumed to occur at two stages: stage I, which is referred to as the energy limiting stage, and stage II, referred to as the falling rate stage. At stage I, evaporation occurs at maximum rates and is limited only by the energy available to the soil surface; thus $K_r = 1$. At stage II, soil water evaporation is assumed to linearly decrease as a function of the remaining soil water content in the topsoil:

$$K_{r,i} = \left(\frac{TEW - D_{e,i-1}}{TEW - REW}\right),$$

where $D_{e,i-1}$ is the water depletion from the soil surface layer on the previous day, $TEW$ is the total evaporable water [$= 1000 \left(0.05 - 0.50z_c\right) z_c$], and $REW$ (8 mm) is the readily evaporable water, defined as the maximum water depth that can be evaporated from the topsoil layer without limitation at stage I. $z_c$ (0.1) is the depth of the near-surface soil layer from where evaporation occurs, whose value depends on the soil texture. The $REW$ and $z_c$ values were tabulated in the FAO-56 bulletin based on the site soil texture.

Soil water depletions at the root system depth ($D_r$) and from the surface layer ($D_e$) were determined by solving the following simplified SWB (Allen et al. 1998; Cammalleri et al. 2013):

$$D_{r,i} = D_{r,i-1} - P_i - I_i + ET_{e,i} + DP_i,$$

$$D_{e,i} = D_{e,i-1} - P_i - \frac{I_i}{f_w} + \frac{E}{f_{ew}} + DP_i,$$

where the subscript I is the end of the present day and i-1 the previous day (mm d$^{-1}$) and DP is the water loss by deep percolation (mm d$^{-1}$) given by:
\[ DP_i = (P_i + I_i) - ET_{c_d} - D_{i-1}, \]  

(26)

### 2.6 Inverse Modeling - Levenberg–Marquardt Method

Apart from determining the single \((K_c)\) and basal \((K_{cb})\) crop coefficients from the ThM and dual \(K_c\) methods, respectively, by adjusting tabulated values (Eq. 9) as described above, we also evaluated these parameters as obtained by inverse modeling. The inverse problem consisted of solving the following objective function:

\[ f(P) = \frac{1}{2} \sum_{i=1}^{N} (ET_a - ET_{a,\beta})^2, \]  

(27)

where \(f(P)\) is the objective function to be minimized, \(ET_{a,\beta}\) is the evapotranspiration obtained by the BREB method, \(ET_a(p)\) is the evapotranspiration estimated by the ThM or dual \(K_c\) model, and \(p\) is a vector containing the parameters to be fitted, which herein corresponds to the \(K_c\) or \(K_{cb}\) parameter for the mid-season growth stage, for ThM (single \(K_c\)) or dual \(K_c\), respectively.

The minimization of Eq. (27) was accomplished by using the Levenberg–Marquardt method, which is a deterministic method searching for deviation initially along the steepest gradient of \(f(p)\) and switching the search gradually to the Gauss–Newton algorithm as the minimum \(f(p)\) is approached. This is performed by adding the term \(\lambda I\) (where \(I\) is the identity matrix) to the diagonal matrix \(J^TJ\) of the resulting system to be solved, making it a positive definite matrix, and making it possible to choose initial candidates for the solution within a wider range of values (Moura Neto and da Silva Neto 2013). At the beginning of the iteration process, \(\lambda\) is taken to be large and then reduced gradually to zero toward the end of the iteration process. The optimization procedures were implemented in Scilab® software.

### 2.7 Statistical Analysis

\(ET_a\) estimated by the ThM or dual \(K_c\) model with adjusted and optimized crop coefficients were compared to the \(ET_a\) determined by the BREB through simple linear regression. The precision and accuracy of the model estimates were determined by the coefficient of determination \((r^2)\) and the modified Willmott index \(d_{\text{m}}\), respectively (Willmott et al. 1985). An estimation of the absolute error was performed by the root mean squared error (RMSE), dividing it into its systematic (RMSE\(_s\)) and non-systematic (RMSE\(_u\)) components.

The means \((\mu)\) for measured \(ET_a\) \((\mu_x)\) and \(ET_a\) estimated \((\mu_y)\) by ThM and dual \(K_c\) method (with the adjusted and optimized coefficients) were compared by Student’s \(t\)-test at \(p<0.05\). The null hypothesis was \(H_0: \mu_x = \mu_y\), and the alternative hypothesis was \(H_1: \mu_x \neq \mu_y\).

### 3 Results and Discussion

#### 3.1 Weather and Soil Water Conditions

In most of the experimental period (96% of days), the SW simulated by the two models with the adjusted FAO56 and optimized crop coefficients was approximately 45 mm,
corresponding to 0.9 of the total available water (TAW = 50 mm) (Fig. 1a). The high SW values were due to the high precipitation that occurred during the evaluated period, with precipitation events occurring every day throughout the experimental period, totaling 373.4 mm. The daily total precipitation varied from 1.0 (161 Day of Year — Doy) to 79.3 mm (158 Doy) (Fig. 1b), corresponding to an average of 14.4 mm per precipitation event. The accumulated ET₀ for the evaluated period was 73.9 mm (average of 2.84 mm d⁻¹), and thus P–ET₀ was equal to 299.5 mm. The daily extremes of ET₀ ranged from 1.6 (158 Doy) to 4.0 mm d⁻¹ (153 Doy). These high precipitation values and ET₀ < 4 mm d⁻¹ were expected since the experiment was carried out during the region’s rainy season, which coincides with the austral winter.

3.2 Bowen Ratio – Energy Balance (BREB)

Applying the data validity analysis criterion proposed by Perez et al. (1999) led to a data rejection of 42% from a total of 618 hourly observations. These results agree with similar percentages of filtered Bowen ratio data from several studies (Perez et al. 1999; Peacock and Hess 2004; Carmo et al. 2017). The highest proportion of rejections was observed at night (Fig. 2a), whereas at daytime, inconsistent data were only observed in the early morning and late afternoon, and all the data at 18:00 local time were filtered. The inconsistency of the BREB at these times is well reported in the literature (Inman-Bamber and McGlinchey 2003; Peacock and Hess 2004; Perez et al. 1999) and is associated with errors in the sensible heat flux sign or with low values of Δe or available energy (Rₙ – G). Most of the rejections at 18:00 local time were caused by errors in the flux-gradient relation, where the available energy was negative (Rₙ – G < 0), with Δe > 0, which by Eq. (5) implies that β should be less than −1. However, β values were within the range −1 < β < 0, which characterized a change in the H sign, not followed by LE.

**Fig. 1** (a) Daily available soil water (SW) simulated by the Thornthwaite and Mather (ThM) and dual Kₑ (dual Kₑ) models, (b) reference evapotranspiration (ET₀) and precipitation as a function of days after planting (DAP)
The distribution of consistent and inconsistent values of $\beta$ as a function of $\Delta e$ is illustrated in Fig. 2b. Thus, as can be inferred by Eq. (6), as $\Delta e$ approaches 0, the data rejection interval is increased for $\beta$ values close to -1. Most of the data rejection occurred for $R_n - G < 0$, usually at night (Fig. 2a), when lower $\Delta e$ values occurred.

The box plots of Fig. 2c summarize the relative uncertainty for LE estimates at daytime for all days from the evaluated period. The larger the box plot size, the greater the variation in the relative LE uncertainty for a given time. The presence of outliers indicates the number of days whose relative uncertainty did not follow the distribution pattern of the values at that time. Overall, the greatest uncertainties in the LE estimates occurred in the early morning and late afternoon. In the early morning, the relative uncertainty in the LE estimate was greater than 100% for more than 50% of the evaluated days. At late afternoon, however, the uncertainties were less than 30%, with some atypical days characterized by the presence of outliers with uncertainties of approximately 45%. For the other daytime hours, the relative uncertainty in the LE estimate was approximately 20%. The LE values in the early morning and late afternoon are considerably low, and therefore, the high relative uncertainties at these times have little impact on the computation of daily evapotranspiration.
3.3 Crop Coefficient - Single and Dual Kc

As the simulated SW was close to TAW during most of the experimental period (SW/TAW > 0.9), the ET determined by the BREB (ETβ) is expected to approach the FAO56 definition of ETc. Therefore, Kc was obtained simply by the ETβ/ETo ratio. The field experimental values of Kc varied between 0.92 and 1.21, with an average of 1.01 (± 0.08) (Fig. 3). There was a strong correlation (r = 0.83) between ETo and ETβ and low dispersion (coefficient of variation – CV = 8%), with only one observation out of the 95-confidence interval of the predictions. Similar correlations were also found by Inman-Bamber and McGlinchey (2003), except that in our case, the intercept of the relationship between ETc and ETo did not show statistically significant differences from zero (t-test, p < 0.05), indicating that the bias was not statistically significant. There were only two upper (Kc > 1.15) and lower (Kc < 0.93) outliers based on the analyzed sample size. However, these values are within the mid-season Kc range (0.93–1.43) observed in several studies (Inman-Bamber and McGlinchey 2003; Marin et al. 2020; da Silva et al. 2012, 2013; Dingre and Gorantiwar 2020).

The Kc,mid in the ThM model retrieved from optimization was equal to 1.05 (only 3% less than the Kc obtained experimentally), whereas the adjusted Kc FAO56 (1.25) was 16% and 19.2% higher than the optimized and experimental Kc, respectively. Discrepancies between experimental and adjusted Kc FAO56 were also found in other studies. For instance, Bastidas-Obando et al. (2017) and da Silva et al. (2013) in a wet climate found lower Kc values compared to the adjusted FAO-56. Conversely, da Silva et al. (2012) found

![Fig. 3 Relationship between daily reference evapotranspiration (ETo) and sugarcane evapotranspiration determined by the BREB method (ETβ) and box plot of the crop coefficient (Kc)](image-url)
a higher average $K_{c\,mid}$ (1.43) for the same sugarcane variety under irrigated conditions in
the first ratoon cycle grown in a semiarid region of Brazil, which was attributed to the high
wind speeds and the semiarid climate of the region.

The optimized $K_{cb\,mid}$ in the dual $K_c$ method from FAO56 was equal to 1.03, that is,
14.2% less than the adjusted FAO-56 value (1.20) for the evaluated experimental weather
conditions. Bastidas-Obando et al. (2017) also found a lower average $K_{cb}$ for irrigated and
non-irrigated sugarcane than adjusted FAO56.

### 3.4 Actual Evapotranspiration Estimated by ThM and Dual $K_c$ x ET – BREB

ET determined by BREB ($ET_\beta$) for sugarcane during the experimental period varied
between 1.54 and 3.91 mm d$^{-1}$, with an average of 2.83 ($\pm$ 0.55) mm d$^{-1}$, whereas ET estimated
by the ThM model with adjusted FAO56 $K_c$ ranged from 2.01 to 4.60 mm d$^{-1}$ (mean
3.48 $\pm$ 0.62 mm d$^{-1}$). The mean ET estimated by ThM with adjusted $K_c$ differed statistically
from the mean $ET_\beta$ by the t-test ($p < 0.05$). The ET estimated by the ThM model with
optimized $K_c$ ranged from 1.69 to 3.91 mm d$^{-1}$, and its average (2.93 $\pm$ 0.52 mm d$^{-1}$) did
not differ statistically (t-test, $p < 0.05$) from the mean $ET_\beta$.

Using adjusted FAO56 $K_c$, the ThM model overall overestimated $ET_\beta$ by approximately
22% ($r^2 = 0.82$), thus resulting in relatively low accuracy ($d_m = 0.44$). The RMSE was
0.69 mm d$^{-1}$ (Table 1), representing 24.4% of the observed average. The highest
RMSE (87.5%) came from systematic error (RMSE$_s$), indicating a need to optimize
the model coefficients. Conversely, although using the optimized $K_c$ in the ThM model did not
improve model precision ($r^2$), it enhanced model accuracy, overestimating $ET_\beta$ by only 2.7%
and lowering RMSE. Accordingly, the contribution of systematic error decreased (7%),
while the fraction of non-systematic error increased (17%).

The time course of $ET_a$ shown in Fig. 4c illustrates how ThM improved $ET_a$ estimation
with $K_c$ retrieved from inverse modeling in contrast with the adjusted FAO56 $K_c$. Additionally,
using optimized $K_c$ did not change the trend pattern of the estimated $ET_a$ over time by
the ThM model, but did improve the proximity to $ET_\beta$ (Fig. 4). Overall, the ThM model
with optimized $K_c$ tended to slightly overestimate $ET_a$ for values lower than approximately
3.5 mm d$^{-1}$ and underestimate $ET_a$ for higher values. The intercept from the linear regression
between $ET_a$ estimated by the ThM model with adjusted FAO56 $K_c$ and $ET_\beta$ was a
statistically significant difference from zero (t-test, $p < 0.05$), indicating bias (Inman-Bamber
and McGlinchey 2003), while the intercept using the optimized $K_c$ was not statistically
significant difference from zero.

Only in two days (DOY 172 and 175) did $ET_a$ simulated by the ThM model with
adjusted FAO56 $K_c$ show smaller differences compared to $ET_\beta$. For these days, the field

| Table 1 | Statistical coefficients for the comparison between ET determined by the BREB method and estimated by the Thornthwaite and Mather (ThM) and dual $K_c$ models, with the adjusted FAO-56 and optimized crop coefficient |
|---------|---------------------------------|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| Index   | ThM                             | Dual $K_c$                       |                  |                  |                  |                  |
|         | Adjusted | Optimized | Adjusted | Optimized | Adjusted | Optimized |
| $r^2$   | 0.82     | 0.82      | 0.83     | 0.82      | 0.83     | 0.82      |
| $d_m$   | 0.44     | 0.88      | 0.44     | 0.79      | 0.44     | 0.79      |
| RMSE    | 0.69     | 0.24      | 0.70     | 0.30      | 0.70     | 0.30      |
| RMSE$_u$| 0.60     | 0.07      | 0.62     | 0.11      | 0.62     | 0.11      |
| RMSE$_u$| 0.09     | 0.17      | 0.08     | 0.19      | 0.08     | 0.19      |
The ET estimated by the dual Kc model with adjusted Kcb FAO-56 varied between 2.01 and 5.03 mm d⁻¹, with an average equal to 3.49 mm d⁻¹ (±0.61 mm d⁻¹), which statistically differed from the average ETβ (t-test, \( p < 0.05 \)). In this case, ET was overestimated on average by approximately 22% (Fig. 5). The RMSE was 0.70 mm d⁻¹, representing 24.8% of the observed average, and the systematic error (87.8%) had a major contribution to the RMSE.

Using optimized Kcb retrieved by inverse modeling, ET values ranged from 1.69 to 4.61 mm d⁻¹, and its average (3.01±0.58 mm d⁻¹) did not differ statistically (t-test, \( p < 0.05 \)) from the average ETβ. Similar to ET estimated by the ThM model, the optimized Kcb did not improve model precision, but did improve model accuracy (Fig. 5a). However, the dual Kc model had a lower accuracy improvement than the ThM model, as seen by the \( d_m \) and RMSE shown in Table 1.
By comparing the ThM model and dual Kc method to each other, we found no statistically significant difference between them (t-test, \( p < 0.05 \)). The \( ET_a \) values for both methods remained close to each other, with \( r^2 \) equal to 0.98 and an RMSE of 0.06 mm d\(^{-1}\), thus showing little difference between the methods. da Silva et al. (2012) compared ET estimates for sugarcane by the single Kc and dual Kc methods with adjusted \( K_c \) and \( K_{cb} \), respectively, to the SWB method and found that the dual Kc method performed better, with high precision and lower normalization. The regression intercepts between measured values and ET were statistically significant for both methods, indicating bias in the estimates.

4 Conclusions

Thornthwaite and Mather’s SWB adapted for crops coupled with the single crop coefficient method (ThM) and the dual Kc method (dual Kc) are simple alternatives to estimate actual evapotranspiration. Crop coefficient for these models (\( K_c \) for ThM and \( K_{cb} \) for dual
Kc) are available in FAO-56 for several crops for each growth stage, as well as an equation to adjust these parameters to local climate conditions. However, some authors have shown that adjusted values can be different from those obtained experimentally, leading to inaccurate evapotranspiration estimates (da Silva et al. 2012; Bastidas-Obando et al. 2017; Marin et al. 2020). Thus, the aim of this study was to assess the performance of the ThM and dual Kc models to estimate daily actual evapotranspiration with Kc and Kcb determined by inverse modeling. The model comparisons and optimizations were performed with ET determined by the Bowen Ratio – Energy Balance method (BREB), and the optimization problem was solved with the Levenberg–Marquardt algorithm (LM). The results presented herein allow us to conclude the following:

(i) The single Kc from the ThM and the Kcb from the dual Kc method can be satisfactorily retrieved by inverse modeling using the LM algorithm based only on ET determined by the BREB. This approach can be a feasible alternative to find crop coefficient parameters, especially Kcb, which is more difficult to obtain as it requires plant transpiration measurements.

(ii) The ThM and the dual Kc methods are precise and accurate for estimating the actual evapotranspiration of sugarcane at full canopy closure when using the optimized mid-season Kc (1.05) or Kcb (1.03). Conversely, the use of adjusted FAO-56 Kc and Kcb leads to an overestimation of sugarcane evapotranspiration for the climate and soil conditions evaluated in our study.

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Availability of Data and Material The observed data used in the present study are available upon the authors’ request.

Code Availability The code of the soil water balance models used in the present study is written in the Open Model software and is available upon the authors’ request.

Declarations

Ethics Approval Not applicable.

Consent to Participate All authors agree to participate in any survey or feedback task.

Consent for Publication All authors agree to provide manuscript for publication to the publisher of the journal.

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