Monitoring water stress using time series of observed to unstressed surface temperature difference

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Abstract

Remote sensing data in the thermal infra red (TIR) part of the spectrum provides indirect estimates of water stress – defined as a function of the ratio between actual and potential evaporation rates – at the earth surface. During the first stage of evaporation (“energy limited” evaporation), this ratio is close to one. During the second stage of evaporation (“soil controlled” evaporation) water stress occurs and as a result this ratio drops below one. Recently, methods using TIR data to monitor stress have shifted from establishing empirical relationships between combined vegetation cover/temperature indices and soil moisture status to data assimilation of surface temperature into complex soil–vegetation–atmosphere transfer models. However, data and expertise are often lacking to widely apply those methods. In this paper we investigate the proof-of-concept of using solely the difference between actual and unstressed surface temperature as a baseline to monitor water stress. The unstressed temperature is the equilibrium temperature of a given surface expressed in potential conditions, computed with an energy balance model. Theoretical, modelling, and experimental documentation of the proof-of-concept are shown for datasets acquired within the frame of two international experiments in semi-arid region. We show that the difference between the observed and the unstressed surface temperatures is almost linearly related to water stress. A sensitivity study is carried out to test the impact of modelling errors on the evaluation of the unstressed temperature. We found that even with inaccurate but realistic values of the surface parameters used to solve the energy balance and compute the unstressed temperature, the observed to unstressed surface temperature difference is still more relevant to detect second-stage processes than the difference between the observed surface temperature and the air temperature. The perspective of using an empirical index based on this difference is also investigated. These results are especially attractive for application based on TIR satellite imagery at a regional scale.

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1. Introduction

Detection of crop water stress is crucial for efficient irrigation water management, especially in semi-arid regions. Water stress, or second-stage evaporation (Levine and Salvucci, 1999), corresponds to the reduction in evaporation due to the limited availability of root zone soil moisture. Water stress results in a drop of actual evaporation below the potential rate. Its intensity is usually represented by a Stress Factor ($S$), which is defined more generally by the complement to one of the actual ($\lambda E$) to potential ($\lambda E_p$) evaporation ratio:

$$S = 1 - \frac{\lambda E}{\lambda E_p}$$

(1)
This factor is equal to zero for energy-limited evaporation (unstressed conditions), and increases towards one for soil-controlled evaporation (water stress conditions).

Water stress can be assessed by measuring evaporation rates, and evaluate potential evaporation using classical methods such as Penman-Monteith or an energy balance model by setting the surface resistance to a minimal value. Measurements of total evaporation ($\lambda E$) at the paddock scale can be achieved with the Eddy-covariance method, but this method is costly and needs well-trained staff to operate and maintain it. For larger scale (1 km and above) there is no observational device to measure routinely evaporation, except scintillometry. Scintillometers can provide estimates of the sensible heat flux for a cross-section of about 10 km (Kohsiek et al., 2002). $\lambda E$ can then be obtained as the residual term of the energy balance equation providing estimates of available energy at the same scale using remote sensing data (Ezzahar et al., 2007). These techniques are not trivial to set up and there is a large place to develop alternative methods for the monitoring of water stress.

Data in the thermal infra red (TIR) is linked to soil moisture and thus to the evaporation flux since the surface temperature is obtained through solving the surface energy balance equation. The use of TIR data to monitor stress can be classified into three broad categories (Courault et al., 2005). For each of these categories described below, TIR data can be combined or not to a surface energy balance model (see Table 1) in order to provide more elaborate information:

1. Using TIR data for an assessment of instantaneous flux patterns:
   a. The first group of methods computes indices based on TIR radiance and a combination of surface reflectances: since index maps can be easily deduced from remote sensing images acquired in thermal and visible bands, these methods are very popular. Amongst such methods, one can mention the Crop Water Stress Index (CWSI: Jackson et al., 1981; Jackson, 1982), the Surface Energy Balance Index (SEBI: Menenti and Choudhury, 1993) or the Water Deficit Index (WDI: Moran et al., 1994; Moran, 2004); these indices are different expressions of the Stress Factor, and have been derived from a surface energy balance model. On the other hand, some indices like the Temperature–Vegetation Dryness Index (TVDI: Sandholt et al., 2002) or the Temperature Vegetation Index (TVI: Prihodko and Goward, 1997) do not rely on any parameterization of the energy balance and can be computed directly from remote-sensing data.

   Stress indices are usually based on either the observed surface temperature itself or the difference between the observed surface temperature and air temperature at screen level (Sepulcre-Canto et al., 2006); they rely upon the assumption that for a given image there are places that evaporate at a potential rate ($S = 0$), and very dry, non-evaporating places ($S = 1$); stress levels are scaled according to the distance between the surface temperature of a given pixel and the minimum and maximum surface temperatures observed on the scene; these extreme values are related to the extreme values of $S$, i.e. 0 and 1; more recent studies also state that for each water stress condition the temperature depends on the amount of bare soil seen by the TIR sensor; the scaling between both extremes of $S$ depends on a second remote-sensing variable representing the vegetation cover fraction, which is usually the Normalized Difference Vegetation Index (NDVI), or the Soil Adjusted Vegetation Index (SAVI); this leads to the classical triangle or trapezoidal shape of the temperature/vegetation cover diagram (Carlson et al., 1994; Moran et al., 1994; Boegh et al., 1999; Moran, 2004; Luquet et al., 2004) with its “cold” (unstressed) and “warm” (stressed) edges. The trapezoid method is often used to derive a spatial pattern of instantaneous stress level for a given TIR/NDVI image (Batra et al., 2006). Since the extreme vegetation and moisture conditions are not always present at the time of acquisition, it is not the most accurate way to represent the space/time variability of the hydric status. The use of time series of WDI

### Table 1

Classification of some methods to assess water stress from TIR data.

<table>
<thead>
<tr>
<th>Method</th>
<th>With an energy balance model</th>
<th>Without energy balance model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Instantaneous retrieval</td>
<td>SEBAL, ALARM, SEBS, etc.</td>
<td>TVI, TVDI, etc.</td>
</tr>
<tr>
<td>Time series analysis</td>
<td>CWSI, SEBI, WDI, etc.</td>
<td>Albedo, $T_s - T_a$, $(T_s - T_a)/R_s$, etc.</td>
</tr>
<tr>
<td>Data assimilation in a state-space model</td>
<td>Simple (thermal inertia only, no water balance involved) or complex (SVAT: water balance involved)</td>
<td>Assimilation of time to stress in water balance models (e.g. SVATsimple)</td>
</tr>
</tbody>
</table>
values computed with an energy balance model appears to be a better alternative to monitor water stress instead of mapping water stress levels.

b. The second family of methods involves a surface energy balance model: surface temperature is used as input to derive the sensible heat flux and obtain \( \lambda E \) as a residual of the energy balance; flux maps are produced whenever an image is available. The first methods do not model explicitly the difference between the aerodynamic and the surface temperatures (Seguin and Itier, 1983; Lagouarde, 1991) whereas most recent methods parameterize this difference (Chehbouni et al., 1997) or provide an estimate of the \( k_B \) parameter (SEBAL: Bastiaensen et al., 1998; SEBS: Su, 2002; ALARM: Suleiman and Crago, 2002). As for the indices mentioned above, some methods assume that on a given image there are places that evaporate at a maximum rate and other areas with no evaporation. To provide time series of \( \lambda E \), extrapolation methods like data assimilation are required to estimate fluxes for dates between two successive cloud-free images.

2. Using time series of TIR observations:

The second category of methods takes advantage of looking at TIR data time series. Amongst them, the first group, which does not involve any surface energy balance model, uses change detection algorithms and is based on the assumption that when the surface enters the “soil controlled” stage (this stage is also named “supply-limited” in some references), there are strong and sudden changes in surface conditions that impact on the surface temperature. For bare soil and short vegetation, Amano and Salvucci (1997) states that “transitions from atmosphere-limited to soil-limited evaporation can be accompanied by either an increase in afternoon surface temperature relative to either air temperature or morning surface temperature, or an increase in land surface albedo”. The first advantage of using such methods is that they are catching the consistency between the evolution of TIR observations and the date of the last irrigation or rainfall event instead of computing instantaneous stress levels independently of the drying/wetting history. The other advantage is that systematic errors in observed surface temperature (constant bias) do not significantly affect the results of stress detection algorithms since the later are only looking at trends in the TIR data time series and not at absolute values. The second type of methods involves a surface energy balance model. Within this category, and amongst the most popular methods to use TIR data to monitor water stress, one can mention the analysis of time series of CWSI interpreted as the evolution in time of the Stress Factor (Jackson et al., 1981; Jackson, 1982). Finally, instantaneous indices can be compared for a limited number of dates with continuous time series of independent water status information: Sandholt et al. (2002) have found a good correlation between TVDI values and the soil moisture maps computed with a distributed hydrological model, whereas Goward et al. (2002) have found a good relationship between time series of TVI and surface soil moisture simulated by a complex soil vegetation atmosphere transfer (SVAT) model.

3. Assimilation of TIR data into land surface models:

Assimilation sensu lato enables to adjust either a state variable or a parameter of a given state-space process model in order to reduce the difference between the simulated and the observed radiometric surface temperatures. Whether the land surface model is based on the integration in time of the surface energy balance (in that case the only state variable is the soil temperature, taking into account the soil thermal inertia, e.g. Castelli et al., 1999) or the integration in time of the water balance (Boulet et al., 2002), or both (Demarty et al., 2004; Olioso et al., 2005), the problem is that model uncertainty, especially on the evaluation of soil thermal or hydrodynamical properties, is large. These methods, while interesting in the preparation of future observing systems (Pellenq and Boulet, 2004), have similar performances as more simple ones cited before (Jacob et al., 2006).

This study addresses possible improvements in the second category of methods, more specifically the use of time series of CWSI/WDI-type indices. The popular CWSI formulation proposed by Jackson et al. (1981) suffers from two major limitations: first, it does not take into account the temporal variability of the canopy structure and extent (Yuan et al., 2004); furthermore, it assumes that the surface and the aerodynamic temperatures are equal. Therefore, as stated by Moran (2004), “Application of CWSI with satellite- or aircraft-based measurements of surface temperature is restricted to full-canopy conditions so that the surface temperature sensed is equal to canopy temperature”. Many other expressions of the Stress Factor are available in the literature. In the case of sparse vegetation or changing vegetation cover, Leaf Area Index can be used to modulate a single-source surface resistance (Moran et al., 1994) while Boegh et al. (2002) uses a decoupling coefficient to retrieve simultaneously an equivalent of
the surface resistance for the soil and for the canopy. In
the “trapezoid” approach, Moran et al. (1994) show
that the Stress Factor can be expressed as a function of
two temperature boundaries in the NDVI versus
that the Stress Factor can be expressed as a function of
space, the unstressed or “cold edge” ($T_{s0}$) and stressed
or “warm edge” ($T_{a0}$) temperatures. This expression is
called the Water Deficit Index (WDI):

$$S = \frac{T_s - T_{sp}}{T_{s0} - T_{sp}}$$  \hspace{1cm} (2)$$

In (2), $T_{s0}$ is the theoretical temperature of a non-
evaporating surface with the same biophysical prop-
ties and climate conditions as the actual. It is calculated
by solving the surface energy balance in actual condi-
tions but replacing $\pm E$ by 0. Computation of $T_{s0}$ is not
trivial, because it corresponds generally to high soil heat
flux values (the soil thermohydric properties are not
easy to evaluate at the appropriate space–time scale) as
well as unstable convective conditions (which rely on
semi-empirical stability functions). Similarly, heat
exchange between the canopy and the soil for sparse
conditions is not easy to evaluate when the soil is hot
and dry but the plant is extracting water from the deep
soil at a near-potential rate. In practice, model un-
certainties in the evaluation of $T_{sp}$ and $T_{s0}$, as well as
measurement errors on $T_s$, can lead to erroneous CWSI/
WDI estimates. Values of CWSI outside the range $[0, 1]$ are
not uncommon (Alderfasi and Nielsen, 2001; Bar-
Bos da Silva and Ramana, 2005), especially in semi-
arid regions where $T_{s0}$ can reach very high values.
Outside of the $[0, 1]$ range, CWSI values cannot be
interpreted as $S$ estimates, and need to be rescaled
accordingly. A practical solution to account for this
discrepancy is to stretch the cold and warm edges
simulated by a SVAT model to the boundaries of the
observed trapezoid (Gillies et al., 1995). However, the
use of the WDI is dependant on how one matches the
“observed” trapezoid that is not always sampling all
vegetation, moisture and atmospheric conditions and the
“simulated” trapezoid computed with an energy
balance model that should be adapted to those varying
vegetation, moisture and atmospheric conditions.
Furthermore, the retrieved stress level depends largely
on the instantaneous shading conditions.

Acknowledging the limitations of the CWSI/WDI
methods, many recent research avenues on stress
detection have gone back to the interpretation of time
series of surface to air temperature difference (Amano
and Salvucci, 1997), or shifted to data assimilation.
However, when data or expertise is lacking to apply
SVAT models, the CWSI or WDI concept may be useful
if it can be improved with the help of the recent
progresses in the description of the surface energy
balance components of SVAT models to provide simple
yet robust stress indices derived from TIR data (Vidal
and Devaux-Ros, 1995). In this study, instead of
deriving a non-dimensional index, we propose to focus
solely on the WDI numerator, i.e. the difference
between the observed temperature and the temperature
in potential conditions ($T_s - T_{sp}$).

The aim of this paper is two-fold: first, to document
the theoretical, experimental and modelling evidences
that the difference between the observed temperature
and the temperature in potential conditions simulated
with little a priori information on the land surface is a
suitable information to monitor water stress under
variable vegetation cover conditions, compared to
classical indices based on observed variables alone
(air to surface temperature difference, albedo, etc.);
second, to assess the impact of model uncertainties on
the accuracy of stress detection when a simple
uncalibrated “big leaf” model is used to estimate the
surface temperature in potential conditions, and rate this
performance on a validation dataset for several
vegetation types and conditions.

The paper is organized as follows: first the simple
“big leaf” energy balance equation is run together with
first guess parameter values to produce unstressed
surface temperature and potential latent heat flux time
series for three water stress periods identified within two
dataset datasets. The evolution of both $T_s - T_a$
and $T_s - T_{sp}$ is then plotted against the observed and the
potential latent heat fluxes to investigate the ability of
both thermal indices to detect stress. Then the
relationships between either $T_s - T_a$ or $T_s - T_{sp}$ and
the Stress Factor $S$ are identified by linearizing the “big
leaf” model. In order to assess the variability of the
linear regression coefficients, a physically-based
reference SVAT model is applied for a wide range
of vegetation and soil moisture conditions, first in
known conditions, then when uncertainty in the energy
balance components is synthetically taken into account.
After this sensitivity analysis, the validity of the average
linear relationship between $T_s - T_{sp}$ and $S$ is checked
against experimental data. Finally, some examples of
application of this relationship are provided in
conclusion.

1.1. Relevance of the $T_s - T_{sp}$ time series in
monitoring stress

Coupling of the energy and the water exchange at the
earth surface is only active when the atmospheric
conditions are not limiting the evaporation process; therefore under most circumstances there is no coupling and actual and potential conditions are identical. While the concept of potential evaporation is widely used in the literature (see Lhomme, 1997, for a review and a discussion of its definition), the concept of “temperature in potential conditions” is rarely used outside complex non-dimensional indices such as the WDI. The difference between the observed and the unstressed surface temperature is, in theory, sufficient to detect stress, but, since $T_{sp}$ is the output of an energy balance model and is therefore prone to model and data errors, its proof-of-concept needs to be investigated. The foreseen advantage of concentrating on this difference is that detecting changes in $T_s - T_{sp}$ time series is easier than for the CWSI/WDI, since both uncertainty sources can be graphically represented: while model errors in the $T_{sp}$ estimate can be deduced from specified parameter uncertainty, TIR observation errors can be deduced from remote sensing radiative transfer studies, independently of $T_{so}$ uncertainties, and also graphically displayed.

### 1.1.1. Experimental evidence: analysis of three water stress events

In this study, two datasets were used: the first one was collected during the SudMed project (Chehbouni et al., 2006) in 2003 over two patches of wheat whose size (4 ha) exceeds the basic fetch requirements: the B123 site under bare soil conditions and at a maximum Leaf Area Index $L$ of 3, and the B27 site with a maximum $L$ of 4; the second one was acquired during the SALSA experiment in 1997 (Goodrich et al., 2000) over a large sparse grassland field at two phenological stages: one at maximum development with a $L$ of 0.8 and the second at senescence with a starting $L$ of 0.5. In both datasets, latent heat flux was measured with a Krypton (B27), a LICOR7500 (B123) or an EDISOL (SALSA) Fast Response Hygrometer and a 3D Sonic Anemometer with an embedded fast-thermocouple. TIR data was acquired with Everest Infra Red Thermometers (IRTs) looking at nadir with a 60° field of view at a height of 2.3 m (SALSA) and 2 m (SudMed). All IRTs have been calibrated using an Everest black body during the experiment and prior to the experiment in a laboratory with an adjustable ambient temperature. Other measurements include in situ classical meteorological forcing, albedo and Leaf Area Index. Experimental set-ups are presented in Boulet et al. (2000) for SALSA and Duchemin et al. (2006) (see also Er-Raki et al., 2007) for SudMed. For each site, stress was assessed by looking at time series of daily averaged observed latent heat flux ($\lambda E$) and simulated latent heat flux in potential conditions ($\lambda E_p$) during dry down periods in between two successive irrigations or rainfall events. $\lambda E_p$ was computed by solving the simple “big leaf” energy balance equation presented in Appendix A for the unstressed surface temperature ($T_{sp}$). Parameter values were taken from the middle of the $a$ priori ranges given in Table 2, which can be considered as “realistic” average values for most continental surfaces. In order to match $\lambda E$ just after an irrigation (SudMed) or a major rainfall event (SALSA), $\lambda E_p$ was multiplied by an adjustment factor (from 0.9 for B27 to 1.1 for B123). This allows for compensating for measurement errors in $\lambda E$ or inaccurate parameter specification in simulated $\lambda E_p$. Sharp divergence of $\lambda E$ from adjusted $\lambda E_p$ time series was interpreted as the starting date of water stress, or “time-to-stress”. Two water stress periods were identified for B123 and SALSA, and one for B27 (see Figs. 1–3Figs. 1a-3a). It corresponds to 6-Mar. (B123 full cover, Fig. 1a), 27-Mar. (B27, Fig. 2a) and 4-Sep. (SALSA maximum cover, Fig. 3a). In parallel, time series of $T_s - T_{sp}$ and $T_s - T_p$ differences at midday were plotted for the

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>Parameter range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Both models</td>
<td>Minimum stomatal resistance</td>
<td>20–200 (s m$^{-1}$)</td>
</tr>
<tr>
<td></td>
<td>Ratio of perturbated to observed Leaf Area Index (also applies for vegetation height)</td>
<td>0.5–1.5 (–)</td>
</tr>
<tr>
<td>“big leaf”</td>
<td>Empirical parameter of the aerodynamic to surface temperature relationship</td>
<td>5–20 (–)</td>
</tr>
<tr>
<td></td>
<td>Mixed surface albedo</td>
<td>0.15–0.3 (–)</td>
</tr>
<tr>
<td>ICARE-SVAT</td>
<td>Momentum to heat roughness lengths ratio</td>
<td>2–20 (–)</td>
</tr>
<tr>
<td></td>
<td>Sand fraction</td>
<td>0–0.4 (–)</td>
</tr>
<tr>
<td></td>
<td>Clay fraction</td>
<td>0–0.3 (–)</td>
</tr>
<tr>
<td></td>
<td>Soil albedo</td>
<td>0.15–0.3 (–)</td>
</tr>
<tr>
<td></td>
<td>Vegetation albedo</td>
<td>0.15–0.25 (–)</td>
</tr>
<tr>
<td></td>
<td>Soil and vegetation emissivities</td>
<td>0.92–0.98 (–)</td>
</tr>
</tbody>
</table>
selected periods. For B123 and B27, both full cover (Figs. 1b and 2b) conditions show a quick increase in $T_s/C_0T_{sp}$ after the time-to-stress but a continuous increase in $T_s/C_0T_{sa}$ before and after the time to stress. $T_s/T_{sp}$ is therefore a pertinent stress indicator in that case. In order to check that the increase in $T_s/T_{sp}$ is not due to senescence but rather to water stress before senescence, trends of other biophysical parameters, albedo and Leaf Area Index, are displayed on Fig. 4. Albedo values show a clear trend after senescence only, i.e. around 16-May, while water stress is present as early as 6-May. For the water stress period identified within the SALSA dataset (Fig. 3), it is not as clear as for SudMed. Both $T_s/T_{sp}$ and $T_s/T_{sa}$ differences increase at the same time, two days after the time-to-stress.

1.1.2. Modelling evidence: linearization of the simple “big leaf” model

Surface temperature in potential conditions can be obtained through several parameterizations, the most
simple being the Penman-Monteith equation (which is at the basis of the CWSI index), the most complex, yet computed in most SVAT models, being the simulated nadir radiometric temperature, which can be computed from different individual temperature components (for example the soil and the vegetation). In that case the soil and the vegetation surface temperatures can be derived by solving a dual-source (Shuttleworth and Wallace, 1985; Kustas and Norman, 1997) energy budget in potential conditions, and setting (1) the soil surface resistance and the stomatal resistance to a minimum value and (2) the soil heat flux to a fraction of the ground net radiation. In this section we will investigate the relationship between both $T_s - T_{sp}$ and $T_s - T_a$ temperature differences and $S$ through the use of the simple “big leaf” energy balance equation. The complexity of this model lies between the Penman-Monteith and the dual-source energy balance expressions, and it can easily be linearized. It compensates for both limitations of the Penman-Monteith expression used in many studies (e.g. Moran et al., 1994; Vidal and Devaux-Ros, 1995): it takes into account the possible changes in vegetation cover conditions, and it relates the surface and the aerodynamic temperatures through an empirical function that depends solely on the Leaf Area Index (Chehbouni et al., 1997). The surface temperature $T_{sp}$ and the aerodynamic temperature $T_{0p}$ in potential conditions are obtained by solving the surface energy balance in potential conditions:

$$R_{np}(T_{sp}) = G_p(T_{sp}) + H_p(T_{0p}) + \lambda E_p(T_{0p})$$  \hspace{1cm} (3)

where $R_n$ is the net radiation, $G$ the ground heat flux, $H$ the sensible heat flux and $T_0$ is the aerodynamic temperature, respectively. Subscript “p” stands for “computed in potential conditions”.

The Stress Factor $S$ can be written after linearization of (3) along $T_a$, as:

$$S = \frac{\lambda E_p - \lambda E}{\lambda E_p} = \frac{\varphi}{\lambda E_p} (T_s - T_{sp})$$  \hspace{1cm} (4)

where $\varphi = 4\varepsilon_o \sigma T_a^3 \zeta (1 - \xi) + \rho c_p \zeta / r_{d0}$ (the definition of all symbols is provided in Appendix A).
Comparing stressed and unstressed conditions yields:

\[ \lambda E_p = \varphi (T_{so} - T_{sp}) \]  

This means that the WDI expression (2) still holds for the "big leaf" formulation.

Since \( T_{so} - T_{sp} = \lambda E_p / \varphi \) is bounded and does not depend on \( S \), there is a pseudo-linear relationship between \( T_s - T_{sp} \) and \( S \).

\( S \) can also be written as a linear combination of \( T_s - T_a \):

\[ S = \frac{\varphi}{\lambda E_p} (T_s - T_a) + \frac{q}{\lambda E_p} (T_a - T_{sp}) \]  

It is also a pseudo-linear relationship.

By looking at Eqs. (4) and (6), it becomes clear that a sharp increase in \( T_s - T_{sp} \) and \( T_s - T_a \) time series can only be interpreted as the starting point of water stress if (1) the dispersion of \( T_s - T_{sp} \) and \( T_s - T_a \) values around \( S = 0 \) is small, and (2) there is a clear and steady rise in temperature difference for low values of \( S \). Comparing (4) and (6) shows that the linear regressions \( T_s - T_{sp} \) versus \( S \) and \( T_s - T_a \) versus \( S \) have the same apparent slope \( 1/(T_{so} - T_{sp}) = \varphi / \lambda E_p \), but that \( T_s - T_{sp} \) reacts more quickly to stress than \( T_s - T_a \); for \( T_s - T_a \), there is an offset in (6) around \( S = 0 \) which is proportional to the difference between \( T_{sp} \) and \( T_a \). For temperate areas, this difference is generally small, but for semi-arid climates, as shown in the previous section, this difference can reach several degrees Celsius. In what follows, we use model simulation to analyse the variability of the slope \( 1/(T_{so} - T_{sp}) = \varphi / \lambda E_p \) and the offsets of the linear regressions between \( S \) and either \( T_s - T_{sp} \) or \( T_s - T_a \).

1.1.3. Modelling evidence: generalization with a complex SVAT model

In order to check the sensitivity of the \( T_s - T_{sp} \) versus \( S \) and \( T_s - T_a \) versus \( S \) relationships for a wide range of soil moisture and vegetation conditions, we used a complex SVAT model as a reference or "benchmarking" tool to generate time series of \( T_s \), \( T_{sp} \), \( E \) and \( \lambda E_p \). This synthetic dataset was simulated with the ICARE SVAT model (Gentine et al., 2007) for four months (February to May) of climate forcing at the B123 wheat crop site under actual and potential conditions (Fig. 5); this dataset is interesting because it spans a wide range of vegetation conditions (a full growing season with \( L \) values between 0 and 3) and soil moisture status (succession of wet conditions after irrigation or rainfall and long drying periods). ICARE is a physically-based soil–vegetation–atmosphere transfer model with a dual-source soil-plant interface and a multi-layer soil module. The energy balance is solved for two sources of radiation and turbulent heat fluxes, the soil and the vegetation. The water and the heat conduction in the soil are solved for soil moisture and temperature profiles using classical diffusion (heat) and convection-diffusion (water) equations (Richards, 1931). A moderate non-automatic calibration of the parameters was undertaken against observed time series of the energy budget \( (R_n, G, H, \lambda E) \) and the water balance (soil moisture at different levels) in order to ensure the realism of the model’s outputs (not shown). This simulation provides time series of a "reference" Stress Factor \( S \) (simulated) and the associated values of \( T_a \) and \( T_{sp} \) computed by running the model with the same input parameters for both actual and potential conditions. By plotting both temperature differences at 12AM against \( S \), one can check that the correlation between \( T_s - T_{sp} \) and \( S \) is much larger than the correlation between \( T_s - T_a \) and \( S \) (Fig. 6). The pseudo-linear theoretical relationships (4) and (6) between \( S \) and \( T_s - T_{sp} \) or \( T_s - T_a \) respectively appear more clearly for \( T_s - T_{sp} \). \( T_s - T_{sp} \) shows a clear trend around \( S = 0 \), contrarily to \( T_s - T_a \) which shows a large scatter of points corresponding to \( \lambda E_p (T_{sp} - T_a)/\varphi \) values around \( S = 0 \) (Eq. (6)). It is quite interesting to see that the relationship between \( T_s - T_{sp} \) and \( S \) is very linear, even though the conditions that prevail throughout the 2003 growing season vary drastically (bare soil, growing stage, maturity, senescence) over a large range of \( S \) values. This means that the slope \( \theta = T_{so} - T_{sp} \) of
the $T_s - T_{sp}$ versus $S$ relationship is very stable across the different surface and atmospheric conditions, and could be represented by an average value for all vegetation, moisture and atmospheric conditions.

1.2. Impact of $T_{sp}$ estimates uncertainty on index robustness

The different terms of $S$ and $T_s - T_{sp}$ in the "reference" simulation presented above reflects the model's consistency in simulating stress. It does not account for uncertainty in $T_s - T_{sp}$ and $T_s - T_a$ estimates, and therefore for possible deviations from the pseudo-linear theoretical relationship due to simulation/model errors or instrumental biases. Errors associated with the evaluation of both TIR indicators falls within these two broad categories:

- measurement errors: georeferencing and registration shifts, sensor accuracy and spectral characteristics, atmospheric corrections, radiative transfer scheme inversion etc can all be responsible for errors in $T_s$ estimates (see Jacob et al., 2006, for a review); spatial interpolation of the climate forcing, including $T_a$ is also a source of error: meteorological forcing is usually taken from nearby climate stations which are not representative of the local climate and surface conditions; eventually, heterogeneity of the vegetation type and cover and other surface characteristics within the radiometric pixel or the instrumental field-of-view makes it difficult to interpret and fully understand the measurements.

- modeling errors: $T_{sp}$ is derived from a model of the energy balance for a given surface. When one uses an energy balance model like the "big leaf" formulation, there are three parameters that are uncertain: (1) the minimum surface resistance to water vapour extraction, (2) the link between the aerodynamic and the surface temperature and (3) the ratio between the soil heat flux and the total net radiation. If a complex energy balance is used, for instance a dual-source expression (e.g. Braud et al., 1995) the most uncertain parameters are usually (1) the minimum stomatal resistance to water vapour extraction, (2) the parameters of the soil resistance to evaporation, and (3) the ratio between the soil heat flux and the total net radiation. Beyond the choice of the model, definition of "potential conditions" itself is not trivial. It is particularly true in the case of sparse vegetation, and, in general for intermediate values of $L$ (growing stages for instance). Because the soil evaporation extracts water from the top soil whereas roots extract water on a larger soil depth, in most cases soil dries first, then the vegetation. Consequently, there are in fact three stages of evaporation for a given surface (Boulet et al., 2004). It is thus difficult to separate the decrease in soil evaporation rate from the vegetation water stress in a given time series of surface temperature. Possible confusion between both phenomena could be partly overcome by looking at directional temperatures (Boulet et al., 2001).

Given this large range of error sources, one could argue that although $T_s - T_a$ is related to stress with an unknown offset $\lambda E_p (T_{sp} - T_s)/\varphi$, $T_s - T_a$ does not depend on energy balance uncertainties (unlike $T_{sp}$), and might still be more relevant to monitoring water stress when $T_{sp}$ is not known with precision. In order to check the performance of $T_s - T_{sp}$ over $T_s - T_a$ as a water stress indicator under uncertain conditions, a second synthetic analysis was performed. In this second analysis, in order to ensure a large uncertainty on $T_{sp}$ estimates, $T_{sp}$ was generated using a different model than ICARE, and many more "reference" cases than above were investigated. $\lambda E_s$, $\lambda E_p$ and $T_s$ were computed with ICARE under the same conditions as above, and instead of obtaining $T_{sp}$ with ICARE, $T_{sp}$ was calculated with the "big leaf" model presented in Appendix A with slightly different surface parameters than the "reference" simulation illustrated in Fig. 6. The "big leaf" model is a good compromise in terms of model complexity between the Penman-Monteith formulation and a dual-source energy balance, and sufficiently different from ICARE to provide a good benchmarking.
estimate of $T_{sp}$ errors. 100 “reference” simulations were produced by ICARE for surfaces randomly chosen according to their physical properties as a deviation to the simulation shown in Fig. 6; this was achieved by perturbing the most sensitive parameters using a randomly chosen set of parameters from a uniform distribution in the predefined intervals of variation (Table 2); then a surface temperature in potential conditions associated to each “reference” run was computed with a different randomly chosen set of parameters, using the very simple “big leaf” model presented in Appendix A (see also Table 2 for the range of parameters used to generate $T_{sp}$ with the “big leaf” model); combining the “reference” $\lambda E$ and $\lambda E_{sp}$ values simulated with ICARE provides a “reference” $S$. Combining the “reference” $T_s$ and its associated $T_{sp}$ generated with the “big leaf” model, provides an estimate of $T_s - T_{sp}$ which can be compared to the “reference” difference $T_{s0} - T_a$. The correlation coefficient of the linear regressions between both temperature differences and the Stress Factor was then computed for each of the 100 random simulations, i.e. the 100 “reference” combinations of $\lambda E$, $\lambda E_{sp}$, $T_s$ simulated with ICARE for 100 random sets of parameters and the 100 associated $T_{sp}$ values simulated with the “big leaf” model for 100 other random sets of parameters. Fig. 7 shows the scatter plot of the correlation coefficient for one versus the other index (that is, the correlation coefficients of $T_s - T_a$ versus $S$ and $T_s - T_{sp}$ versus $S$ linear regressions). Even when there is a large uncertainty on modelled $T_{sp}$, $T_s - T_{sp}$ is still a more accurate indicator of stress than $T_s - T_a$. It is graphically evidenced on Fig. 7 by locating most (all except two) points under the [1:1] line. Linear regression coefficients are high enough to assume that even in uncertain conditions $T_s - T_{sp}$ can be used to monitor water stress.

1.3. Identification, robustness and generality of the $S \approx (T_s - T_{sp})/\theta$ relationship

We have previously pointed out the need to look at time series of stress levels derived from TIR-based indicators to check their coherence with the irrigation and rainfall temporal patterns. For that purpose, we have shown in section A that isolating trends in $T_s - T_{sp}$ time series is relevant to stress detection. Moreover, it has been shown in the section B that $T_s - T_{sp}$ is almost always linearly related to $S$. It is therefore interesting to check if the empirical value of the slope of the pseudo-linear relationship obtained for the “reference” run ($S \approx (T_s - T_{sp})/10$, see Fig. 6) is robust and general enough to infer $S$ instantaneously. This would provide a more simple index that could be used in place of a WDI. We must recall that according to (4) the denominator $\theta$ corresponds to the difference between the stressed and the unstressed theoretical temperatures $(T_{s0} - T_{sp})$ in given climatic conditions and for a given surface. Using an index of the form $(T_s - T_{sp})/\theta$ to infer the Stress Factor implies that $\theta$ is effectively stable for the whole range of $S$ values. To do so, two conditions of the classical “split-sample” analysis are verified: (1) $\theta$ can be identified (i.e. it can be inferred for a given site during a calibration period), (2) its value must be robust (i.e. its performances in simulating stress for this site do not decrease in a validation period).

In order to check the existence of a quasi-constant $\theta = T_{s0} - T_{sp}$ value, the slope and offset of the linear regressions of $T_s - T_{sp}$ versus $S$ for the 100 simulations presented in Fig. 7 were analysed; the mean and standard deviation for the offset are $-0.15$ and $0.14^\circ C$, respectively, while for the slope it is $10.2^\circ C$ and $1.7^\circ C$, respectively. These rather small standard deviations give us confidence in using $S \approx (T_s - T_{sp})/10$ as a rough but relevant estimate of $S$. In order to validate this relationship, a dataset collected during the growing season 2004 at the B124 field adjacent to B123, was used. $\lambda E_{sp}$ and $T_{sp}$ time series were calculated with the “big leaf” model presented in Appendix A, and the middle value of each parameter range as given in Table 2. It was combined with observed $\lambda E$ and $T_s$, respectively, to produce two estimates of $S$: the first is computed as $S = 1 - \lambda E/\lambda E_{sp}$, the other is obtained from

![Fig. 7. Correlation coefficients of surface to air temperature difference ($T_s - T_a$) vs. Stress Factor ($S$) and actual to unstressed surface temperature difference ($T_s - T_{sp}$) vs. $S$ linear regressions. $T_s$ and $S$ are simulated by ICARE while $T_{sp}$ is simulated by the simple “big leaf” model for the B123 site dataset.](image-url)
Fig. 8. Temporal evolutions of both estimates of Stress Factor for the B124 wheat site together with rainfall and irrigation: the observed Stress Factor $S = 1 - \frac{LEobs}{LEp}$ ($LE$ is the actual observed evaporation rate, $LEp$ is the potential evaporation rate computed with the simple “big leaf” model) and the empirical relationship $S \equiv (T_s - T_{sp})/10$ (where $T_s$ is the observed surface temperature measured by the thermoradiometer and $T_{sp}$ the unstressed surface temperature computed with the simple “big leaf” model). The dashed rectangle shows the period for which the largest discrepancy between both estimates could be in favour of the empirical relationship: the low values around $S = 0$ are consistent with the number of rain events in that period.

the empirical relationship $S \equiv (T_s - T_{sp})/10$. Note that the former cannot be seen as an exact “observed” $S$ since $\lambda E_p$ was not adjusted to match observed $\lambda E$ after rainfall and irrigation (unlike Figs. 1–3) but evaluated using the average of the parameter range given in Table 2. Results are shown on Fig. 8 together with daily amounts of irrigation. 2004 is a much wetter year than 2003, with little stress, and $L$ peaks at about 4.2 around 1-April, while bare soil conditions prevail at the beginning (1–30 January) of the observation period. Vegetation is senescent at the end (10–30 May) of this period. $S$ in bare soil and senescence conditions was well reproduced, while water status of some phenological stages, namely the growing and the end of maturity were less well reproduced (dotted grey box of Fig. 8). Several periods of increase in $S = 1 - \lambda E/\lambda E_p$ can be detected for periods of no-rain or no-irrigation (grey arrows of Fig. 8); they correspond roughly to an increase in $S \equiv (T_s - T_{sp})/10$ with similar slopes, but a bias appears during early growth. $S = 1 - \lambda E/\lambda E_p$ is possibly overestimated for that stage given the number of rainfall events between 20-February and 10-April. This can be due to either an underestimation of $\lambda E$ (as indicated by the poor energy balance closure observed at that time) or an overestimation of $\lambda E_p$. Note that $T_s - T_{sp}$ is always slightly positive, which means that measurement ($T_s$) and model ($T_{sp}$) errors are either small or compensate each other. It is an encouraging result, which would allow us to monitor water status over wheat in that region using thermal images cross-calibrated with our network of in situ IRTs.

Eventually, one could assume that the $S \equiv (T_s - T_{sp})/\theta$ index could be used for many other herbaceous types of vegetation than wheat. In order to extrapolate this index to other surface types, data corresponding to Figs. 1–3 as well as two other similar events mentioned earlier (B123 bare soil and SALSA senescent vegetation) have been gathered into a single data frame to produce a scatter of points in the $T_s - T_{sp}$ versus $S$ space. This dataset spans a wide range of surface types and vegetation water status. The determination coefficient of the $S$ versus $T_s - T_{sp}$ linear regression is 0.57; its slope is 12.9 °C which is higher than the average value found for our wheat site and at the upper edge of the range of values obtained in the 100 simulations; moreover, there is an offset of 2.3 °C. The generality of an average $\theta$ value is thus questionable, and this last exercise should be carried out with more data.

2. Conclusion

Data in the thermal infra red spectrum is still nowadays the most promising data source to monitor water stress at most scales ranging from the paddock to the region. The Crop Water Stress Index proposed by Jackson et al. (1981) expresses the Stress Factor $S$ with TIR data but is not valid for all surface conditions because of its simplifications on the energy balance. More recent methods to study water stress with the help of TIR data have shifted away from the $S$ concept to more complex instantaneous diagrams based on surface cover or complex mathematical methods such as data assimilation. However, the unstressed limit of latent heat flux identified by an unstressed temperature can help the modeller as much as the experimentalist to detect and monitor water stress. For the modeller, there are two potential applications of this study:

1. $T_{sp}$ should be equal to $T_s$ just after a major rainfall event or large irrigation; adjusting the most sensitive parameters of the soil–vegetation–atmosphere interface (i.e. the system of equations of the surface energy balance) in order to reduce the $T_s - T_{sp}$ difference during the first stage of evaporation could lead to an evaluation of several parameters of the energy budget, including the minimum resistances, or the ratio.
between the roughness lengths for momentum and sensible heat, or testing whether in unstressed conditions the atmosphere is always near-neutral; this should allow us to get rid of biases in this period more efficiently than assimilating \( T_s \) at any time.

2. Since \( T_s - T_{sp} \) increases sharply when the surface enters the second stage of evaporation, trend analysis can be used to assess the starting point of this second stage. Time-to-stress depends on water diffusion in the soil; knowledge of the time-to-stress can thus be used to assess the soil hydrodynamical properties, or the equivalent parameterization of stress in more conceptual models. In models like SVATsimple (Boulet et al., 1999), time-to-stress is analytically related to the hydrodynamical parameters, the initial water content and \( \lambda E_p \). Hydrodynamical parameters can thus be analytically inverted from time-to-stress, initial water content and \( \lambda E_p \) estimates, which saves complex calibration procedures in a data assimilation prospective (Demarty et al., 2004): if \( \lambda E_p \) is correct, then one can concentrate on hydrodynamical parameter estimation during the second stage of evaporation, contrarily to classical “automatic” assimilation schemes, which use \( T_s \) directly as an input at all time.

For the experimentalist, the generality of simple empirical indices of the form \( S \propto (T_s - T_{sp})/\theta \) is a promising research avenue. Simple models such as the one presented here could be used to derive \( T_{sp} \). It could be interesting as well to test its performance for a wider range of vegetation types, such as clumped grass, or be interesting as well to test its performance for a wider range of vegetation types, such as clumped grass, or small shrubs, and to very heterogeneous terrains, prior to its application at larger scales.

Finally, this proof-of-concept is supporting the interest for satellite mission proposals such as IRSUTE (Seguin et al., 1999) that would provide estimates of the surface temperature with a typical daily revisit period. Indeed, with current satellite revisit capabilities at the \( \sim 100 \) m pixel resolution (a resolution compatible with most agronomical applications), successive acquisitions of TIR images are interspaced with large periods of time (\( \sim 15 \) days) which can include several rainfall events. Some satellites offer a higher revisit frequency, but for a much coarser resolution (of the order of 1 km) often incompatible with the scale of application. Therefore, using radiation fluxes, albedo, emissivity, and LAI values deduced from the existing frequent (every 2–3 days) high and low resolution Remote-Sensing data would help to derive maps of unstressed temperatures only if it could be combined with series of observed surface temperature images from a high-resolution IRT sensor such as IRSUTE. Then, estimates of pixel-to-pixel water stress levels could be derived with the proposed method once a proper \( \theta \) value is specified.

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Appendix A

The Simple “big leaf” energy balance model (Boulet et al., 2000).

\[
T_{sp} = \frac{\left[ \left( 1 - a_0 \right) R_s + \sigma T_s^4 - T_{sp}^4 \right] \left( 1 - \xi(L) \right)}{\rho c_p \xi \left( \frac{T_{sp} - T_s}{r_s(T_{sp})} \right) + \rho c_p \frac{\left( e^4 \left[ T_0(T_{sp}) \right] - e_0 \right)}{r_s(T_{sp}) + r_s(L)}}
\]

where \( \rho \) is the air density, \( c_p \) is the specific heat of air at constant pressure, \( a_0 \) is the surface albedo, \( R_s \) the incoming solar radiation, \( e_0 \) the surface emissivity, \( e_0 \) the air emissivity, \( \sigma \) the Stefan–Boltzman constant, \( T_s \) the air temperature, soil heat flux \( G \) is a fraction \( \xi(L) \) of the net radiation \( R_n \) depending on the Leaf Area Index (\( L \)), \( T_0 \) is the aerodynamic temperature, \( \xi = (T_{0}\text{op} - T_s)/(T_{sp} - T_s) = (e - 1)/(e^{u/(v-L)} - 1) \) relates \( T_0 \) to the surface temperature \( T_{sp} \) according to \( L \) and an empirical parameter \( u \) (Chehbouni et al., 1997), \( r_s = r_{ad}(1/(1 + R(R(T_{0}\text{op} - T_s))^2) \) is the aerodynamic resistance relating the aerodynamic resistance without stability correction \( r_{ad} \) to the Richardson number \( Ri \) which is a function of the \( T_{sp} - T_s \) difference, \( \eta = 0.75 \) in unstable conditions and \( \eta = 2 \) in stable conditions, \( e^* \) is the saturation vapour pressure at a given temperature, \( e_0 \) is the current air vapour pressure.

\[
r_s(L) = \begin{cases} r_{\text{min}} L & \text{if } L < 1 \\ r_{\text{min}} / L & \text{if } L \geq 1 \\ \end{cases}
\]
is the surface resistance and $r_{\text{min}}$ the minimum stomatal resistance.

One can note that with the above notations $\lambda E_p = \frac{e_f}{g} \left( (e^* (T_0 (T_s)) - e_f) / (r_s (T_s) + r_a (L)) \right)\).

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