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Department of Food Engineering and Agricultural
Equipment, Agroforestry section

Operational tools and applications of EO satellite data to retrieve surface fluxes in semi-arid countries

Maliko Tanguy

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Operational tools and applications of EO satellite data to retrieve surface fluxes in semi-arid countries

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Maliko Tanguy

Directors:
Dr. Alain Baille
Dr. Victoriano Martínez Álvarez

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Fdo.: Alain Baille

Fdo.: Victoriano Martínez Álvarez

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Operational tools and applications of EO satellite data to retrieve surface fluxes in semi-arid countries

Research objectives

The overall objective of the thesis is to develop and evaluate useful tools and applications of Earth Observation (EO) satellite data to estimate surface fluxes in semi-arid countries.

The first specific objective (Chapter 4) is to assess the performance and robustness of the triangle method, a remote sensing (RS) based method to retrieve and map land evapotranspiration (ET). Emphasis is put on the estimation of soil heat flux (G), which represents an important sink of energy in these regions. Estimating accurately G is still very problematic, because of its dependence on both vegetation cover fraction and soil physical properties.

To that aim, the partial goals are:

- Proposal of a new parameterisation scheme for G, based on a linear relationship with the evaporative fraction (EF)
- Assessment of the ET retrieval triangle method with the new G-parameterisation

As a second specific objective (Chapter 5), the triangle method was compared with predictions supplied by a land surface model (JULES) with the purpose of illustrating how these two different approaches can be combined to improve the estimations of surface fluxes.

The third objective is to demonstrate the potential of RS-based information for actual operational applications related to the monitoring of surface fluxes in semi-arid countries (Chapter 6). The first one is the application of the triangle method to obtain maps of actual ET in western Africa. The second one is the application of the same method to analyse the annual evolution of surface energy balance (SEB) components and to study

drought climatology over a 12-year period in the Segura river basin in South-East Spain. The third is the use of sea surface temperature (SST) coupled to an energy balance model of a water body to characterise the thermal behaviour of coastal lagoon (Mar Menor) located in South-East Spain.

Research Highlights

- We assess the performance of a new parameterisation scheme of ground heat flux (G) to be used in remote sensing ET estimation methods (Chapter 4).
- The estimates provided by the new G-parameterisation are compared with AMMA flux. It is shown to perform well, providing improved estimates of sensible heat flux (H) and ET with respect to other G parameterization schemes (Chapter 4).
- The triangle method was compared to ET estimated by means of a land surface model (JULES, Chapter 5). An attempt was made to calibrate JULES using the triangle method through Monte Carlo simulations, but the two methods supply rather different results, indicating that further intercomparison tasks should be carried out to assess the performance of RS-based algorithms and land surface models in estimating the components of the land surface energy balance.
- ET-Mapping using the triangle method provides more insight on the spatio-temporal behaviour of surface fluxes and their response to the African monsoon influence in Sahelian regions (Chapter 6).
- We apply the new G parameterization scheme proposed in Chapter 4 to retrieve and analyse the long term evolution (2000-2011) of the surface energy balance components, G, R_n , H and ET at several sites of the Segura Basin (S-E Spain) using MODIS-Terra data (land surface temperature and NDVI). Temporal and spatial distribution of evapotranspiration reveals different controls on ET (Chapter 6), which was mainly controlled by rainfall in two sites, and by irrigation in the third one.
- MODIS-Aqua Sea Surface Temperature (SST) is used to validate a mathematical model to retrieve surface fluxes in a Mediterranean coastal lagoon (Mar Menor, S-E Spain) (Chapter 6).

Chapter 1: Introduction

1.1. Context of the study

Knowledge and prediction of energy partitioning at the land surface is of primary importance in many issues related to the impact of land use on water resources and climate, desertification processes and land productivity, among others. In particular, evapotranspiration (ET) is an important component of the surface energy balance (SEB), whose knowledge is of high interest for the abovementioned issues. Globally, it is estimated that around 60-80% of the precipitations that falls over land is returned to the atmosphere via ET (Tateishi and Ahn 1996). This proportion may be higher in dry areas, such as the Mediterranean basin or semi-arid regions of the African Sahelian belt.

ET is a necessary input to global climate and hydrological models, and a direct output for applications to irrigation scheduling and agricultural water management. It is a key mechanism for the primary production of vegetation canopy and acts as a regulator of biodiversity over land. In fragile ecosystems such as in arid and semi-arid regions, with scarce water resources and intensification of drought events, adoption and fostering of suitable rainfed/irrigation practices are of paramount importance to maintain the balance between water demand and water resources (Hernandez and Uddameri 2010; Berbel et al. 2010; Elshorbagy 2000; Al-Weshah 2000). In these areas, characterising the spatial and temporal changes in ET constitutes valuable information to be used and integrated into early warning systems and water management tools (Hellegers et al. 2009; Boken 2009; Zschau and Küppers 2003). Information on the time and spatial distribution of ET is also relevant for analyzing climate processes, forecasting weather, studying soil salinisation, assessing aquifer recharge. However, reliable spatial averages of surface energy balance components are difficult to obtain without an extensive meteorological/hydrological measurement system. Punctual ground measurements (i.e., pan-measurement, Bowen ratio, eddy correlation system, weighting lysimeter, scintillometer, sap flow) do not provide accurate information for large areas, especially when these are not homogeneous (Li et al. 2009).

Up to day, many works in areas such as hydrology, climate processes, weather forecast, among others, suffer from inaccurate descriptions of evapotranspiration. Indeed,

ET is difficult to assess in space and time because it depends on the water status and the energy processes at the Earth surface which are highly variable, since they depend on land use, distribution of rainfall and irrigation supply, soil properties and climatic factors, among others. Scientists have been conscious of this problem since the early 90's, and substantial progress has been made since that time, especially in developing algorithms for mapping ET from remote sensing data, in particular using thermal infrared data, some of them specifically targeting agricultural water management issues (Gowda et al. 2008).

There are several methods for estimating water requirement for irrigation management (e.g. FAO56 method, Allen et al. 1998). Modelling studies have also addressed this issue, for example based on the use of the Penman-Monteith equation or on an explicit resolution of the energy balance, the latter in general associated with the soil water balance. However all these methods suffer from the difficulty to access to spatial and temporal variability of the determinants of evapotranspiration, especially quantities describing

- energy exchanges (albedo, surface roughness, ...)
- atmosphere status (air temperature, wind speed, incident radiation, rainfall, ...)
- soil water status (soil moisture, permanent soil characteristics such as parameters of hydrodynamic properties...)

Currently, there are two widely accepted approaches for mapping surface fluxes over large areas, sometimes in combination. They are reviewed in details in Chapter 2.

1. Remote sensing (RS) based methods

RS data provided by optical sensors on board of satellites are extensively used to estimate the spatial distribution of SEB components, by retrieving them from specific algorithms based on the closure of the energy balance equation:

$$R_n - G - H - LE = 0 \quad (1)$$

where R_n is the net radiation, LE is the latent heat flux corresponding to the evapotranspiration process (soil + vegetation), H is the sensible heat flux and G is the soil heat flux. In Eq.1, the heat storage by the aerial part of the vegetation and the energy used in metabolic processes are assumed to be negligible.

Remote sensing techniques have been proposed for ET-mapping, in particular through the use of thermal infrared measurements that provide access to the energy

status and the water status of the surface. Different attempts have been made since the 60's for estimating evapotranspiration using remote sensing approach.

Remote sensing data may be directly introduced in semi-empirical models to compute ET. For example, the simplified relationship, firstly derived at field scale by Jackson et al. (1977) and later analysed by Seguin and Itier (1983), has been used all over the 80's and the 90's for mapping daily ET over large areas (e.g. Lagouarde 1991). In this method, as in the residual method (Norman et al. 1995; Olioso et al. 1999; Brown and Rosenberg 1973; Zhan et al. 1996; Chehbouni et al. 1997), ET is derived from the estimation of net radiation, ground heat flux and sensible heat flux using surface radiation balance and surface energy balance equations together with remote sensing estimates of surface temperature in the thermal infrared domain. Many RS-based methods are derived from the residual method, such as the widely used SEBAL (Bastiaanssen et al. 1998b) and METRIC models (Allen et al. 2005).

In some other models, more realistic representation of the resurface processes is available, as in TSEB (Two Source Energy Balance, Melesse, Nangia, 2005; Norman et al., 1995; Kustas et al., 2003) which separates the contribution to ET from bare soil and vegetation; or multilayer models (Meyers and Paw U 1987; van de Griend and van Boxel 1989; Bruckler and Witono 1989; Braud et al. 1995; Norman 1979).

Another class of RS-based methods are the so-called "graphical methods" such as the triangle method (Jiang and Islam 2001) or S-SEBI (Simplified Surface Energy Balance Index, Roerink et al., 2000). These are based on the graphical interpretation of the relationship between the different remotely sensed properties of the surface (LST and NDVI in the case of the triangle method, and LST and albedo in the case of S-SEBI), which is believed to have a direct connection to surface fluxes.

Many authors acknowledge that remote sensing technology is the most appropriate mean to map regional- and meso-scale patterns of ET on the Earth's surface in a globally consistent and economically feasible manner (Li et al. 2009; Caselles et al. 1992; McCabe and Wood 2006; Kustas and Norman 1996).

2. Land surface models (LSM)

Land surface models (LSMs), or surface vegetation-atmosphere transfer (SVAT) models, is the other approach to predict the components of the SEB (Eq.1). These are fully deterministic models which include a detailed description of the processes regulating evapotranspiration alongside with other biophysical processes taking place at the land surface. These models have been widely developed since the middle of the 90's in

particular in the frame of the development of weather forecast and climate models. In such models, energy balance equations are readily solved providing surface temperature as a solution of the equation system. Conversely to semi-empirical approaches, LSMs give access to a detailed description of soil and vegetation canopy processes, and not only to a limited number of final variables such as evapotranspiration. They simulate intermediary variables linked to hydrological or physiological processes (Oliosio et al. 1999).

LSMs have been mostly designed as surface parameterisations of atmospheric models in order to account for the mass and energy exchanges that occur between the Earth surface and the atmosphere above (e.g. Dickinson et al. 1986; Noilhan and Planton 1989; Sellers et al. 1996). They were also developed for analysing the impact of climate on plant and soil water processes in various environments, for example in relation with canopy microclimate, carbon assimilation processes or water extraction by the plants (e.g. Zur and Jones 1981; Braud et al. 1995; Oliosio et al. 1996; Tuzet et al. 2003). These models describe the exchanges between soil, plant and atmosphere according to the physical and physiological processes occurring in each compartment with generally a fine time step (less than one hour). The use of LSMs over large areas is limited by our ability to provide them with the required input variables and parameters concerning atmospheric, soil and plant characteristics (such as soil moisture, soil hydrodynamical properties, aerodynamic roughness, leaf area index, etc.).

3. Data assimilation

There is also the possibility to combine both approaches, through *data assimilation*, using RS data to improve LSM performance. This can be done broadly in two ways:

Calibration

RS data are used in order to calibrate unknown input parameters of the LSM. One way of doing this is through Monte Carlo Simulations, which consists in repeating random sampling of input parameters in order to solve a mathematical or physical system. In other words, thousands of simulations of the LSM are run with each simulation being made with a different set of input parameters. The set of input parameters that minimises the difference between the solution given by the LSM and remote sensing data is then identified.

Another way of calibrating the LSM using RS data is using the so called “Adjoint-to-the-model” technique. In the Adjoint method (in the following A-method or A-model), an objective (“cost”) function is identified (for example, the weighted error when

comparing observed RS measures with estimated values from the model), and is minimised. This is done evaluating the “cost” function through a forward integration, and subsequently, a “backward” integration of the A-model returns the gradient, or sensitivity, of the cost function with respect to a given set of control variables. To create an A-model implies an important programming effort in the beginning, but once the A-model is working and validated, it usually requires much less computational time than using the Monte Carlo method or another calibration method.

Correcting the model when observation is available

Rather than retrieving model parameters or initial conditions, other methods consist in correcting the model variables by comparing them to remote sensing measurements each time they are available (François et al. 2001; Reichle et al. 2002b; Pipunic et al. 2008).

In these data assimilation techniques, the observed information is accumulated into the model state by taking advantage of consistency constraints with laws of time evolution and physical properties (Bouttier and Courtier 1999). They have been widely developed in meteorological sciences for introducing observations in the atmospheric models used for numerical weather prediction (Talagrand and Courtier 1987). Different methodologies and mathematic tools, such as Kalman filter (Kalman 1960), have been developed for implementing assimilation procedures. Their use for assimilating data in SVAT is just at its beginning (Reichle et al. 2002b; Margulis and Entekhabi 2003a; Judge et al. 2008). However, in most cases the problem is under-determined because data is sparse and only indirectly related to the model variables. The problem is generally of a highly nonlinear nature and the true algebraic solution does not exist. Hence, robust approximate iterative solutions are required to solve the problem.

1.2. Objectives of the study

Given the current context of global concern for climate change (CC) and more particularly, for assessing CC impacts in arid or semi-arid regions facing desertification processes, water scarcity problems and threatened fragile ecosystems, the importance of estimating accurately the spatiotemporal evolution of surface fluxes is more than justified for a wide range of operational applications (agriculture, water management, weather forecast, hydrology, among others).

In light of the present state-of-the-art for methods used to represent spatiotemporal surface fluxes evolution, remote sensing techniques offer a real potential in achieving this goal, and is a valuable alternative or complement to LSMs.

The general objective of this PhD thesis is to exploit this potential of RS techniques for the development of operational tools to estimate surface fluxes in semi-arid countries.

Chapter 2 starts with the state-of-the-art of methods to retrieve surface fluxes, focusing mainly on RS-based methods. It is followed by a description of the main traits shared by most LSMs. The Chapter ends with an overview of the main data assimilation techniques that use RS data.

Chapter 3 is the section dealing with “Material and Methods”. First, a description of the three study sites (AMMA sites, River Segura Basin sites and Mar Menor lagoon) and collected ground data is provided. Then, the RS data used in this work and the image processing are presented. At last, the RS-based method to retrieve ET (triangle method) and the LSM (JULES) that were selected and tested in this work are described in details.

Chapter 4 addresses one of the specific objectives of the PhD thesis, i.e. the proposal and evaluation of a new parameterisation scheme for the estimation of the soil heat flux (G) within RS-based retrieval methods. G is particularly important in semi-arid countries, as it can reach very high values especially during the dry season, and can lead to large errors in the estimation of the other surface fluxes if not correctly estimated. This scheme proposes a novel approach to tackle the problem of accurately estimating G , which is defined in the proposed model as a function of both R_n and EF (evaporative fraction)

estimated from remote sensing. The new scheme is assessed against ground flux data at the AMMA sites to test its performance (accuracy and robustness).

In Chapter 5, a comparative analysis of the triangle method with the LSM JULES is carried out, with the objective of proposing a calibration method for the LSM using ET-estimations provided by the triangle method. Advantages and limitations of the proposed method are discussed. A sensitivity analysis for different input parameters of the LSM is performed. This chapter aims to illustrate how the surface fluxes estimation can be improved by combining the two types of approach.

Three actual operational applications of RS for the retrieval of surface fluxes are presented in Chapter 6. They are proposed as illustrations of functional applications based on RS-techniques and tools to estimate surface fluxes in semi-arid countries.

The first two applications are based on the triangle method. The first consists in generating ET-maps over an arid area under monsoon influence in Western Africa, and in their further analysis. The second deals with the climatology of surface fluxes and the characterisation of the annual pattern of EF and components of the surface energy balance (SEB) at three sites located in a semiarid area of the South of Spain (Segura River Basin), using a 12-year time series of MODIS-Terra data (2000-2011). The third application is the use of Sea Surface Temperature (SST) data from MODIS-Aqua to validate an energy balance model for the Mar Menor Lagoon, in South-East Spain.

Chapter 7 concludes the manuscript with the synthesis of the main results and findings, and a prospective analysis for future development of EO satellite operational applications and tools.

Chapter 2: State-of-the-art

2.1. Introduction

In the 1950s and the 1960s, ET from land surface was thought to be mainly controlled by meteorological conditions, and little attention was paid to spatial changes in vegetation and soil properties. In the 80s, the spatial and temporal dynamic feedback between ET and land surface started to be represented in models that were able to account for atmospheric demand, surface radiation budget, water availability and a range of biological and physical interactions (Kalma and Calder 1994). Accurate point measurement techniques (Bowen ratio, eddy correlation equipment, pan-measurement, weighing lysimeter, scintillometer and sap flow measurements) helped improving understanding and describing local ET processes. However, because of surface heterogeneity, these local measurements can rarely represent heat transfer processes in a reliable way over large areas (French et al. 2005). At about the same period, the use of RS techniques by the land surface scientific community started to spread, and with it, the intent to develop effective methods for determining spatiotemporal estimations of ET.

Since the 80s, numerous RS-based methods to retrieve ET have been proposed, and a few major reviews report on such methodologies from different perspectives. Carlson (1986) reviewed a range of methods that combine the surface energy balance equation with remotely sensed LST. Moran and Jackson (1991), Kustas and Norman (1996) and Quattrochi and Luvall (1999) focused on methods using thermal infrared radiation (TIR) data. In recent years Overgaard et al. (2006) addressed the use of remote sensing from a hydrological perspective, whereas Gowda et al. (2007) and Glenn et al. (2007) focused on estimation approaches with particular reference to plant sciences, agronomy and irrigation applications.

The main methods to retrieve ET from remote sensing have been summarized by Verstraeten et al. (2008) and Li et al. (2009), outlining the theoretical assumptions, advantages and limitations of each of them. Kalma et al. (2008) offer a comprehensive survey of published methods known to date, pointing out the main issues and challenges to address in the future.

In the 70s, just before the RS techniques started to be used by the land surface community, the first generation of LSMs and SVAT models appeared to address the problem of estimating mass and energy exchanges between the surface and the atmosphere. While RS techniques were gradually adopted by the land surface community in the 80s and 90s, LSMs were gradually improved, growing in complexity and in fidelity in describing the biophysical and biochemical processes taking place at the surface.

In the past twenty years, data assimilation techniques have been developed in meteorological sciences for introducing observations in the atmospheric models used for numerical weather prediction (Talagrand and Courtier 1987). Data assimilation technique is the process in which all available information is used in order to estimate objective variables as accurately as possible. Data assimilation in LSMs and SVAT is just at its beginning (Reichle et al. 2002b; Margulis and Entekhabi 2003a; Judge et al. 2008).

This Chapter begins with the presentation of the basic equations and required inputs for estimating ET in a RS context, followed with an overview of the main RS-based methods to retrieve ET. The next section gives a general outlook on the evolution of LSMs over the past decades. The final section briefly introduces some of the most common techniques of data assimilation into LSMs. Each section points out the main advantages and drawbacks of the different approaches.

2.2. RS-based ET-retrieval methods

2.2.1. Basic equations and required inputs for computing evapotranspiration (ET) in a remote sensing context

When investigating energy and water exchanges between the Earth surface and the atmosphere above, evapotranspiration corresponds to latent heat flux (LE) which is related to other energy fluxes by the energy balance equation (Eq. 1 from Chapter 1, section 1.1, page 14).

The net radiation, R_n , represents the available radiative energy for surface processes. It depends on solar radiation (R_g), incident atmospheric radiation (R_a), surface albedo (α_s), surface emissivity (ϵ_s) and surface temperature (T_s):

$$R_n = (1 - \alpha_s)R_g + \epsilon_s R_a - \epsilon_s \sigma T_s^4 \quad (2)$$

σ is the Stefan-Boltzmann constant ($4.903 \cdot 10^{-9} \text{ MJ K}^{-4} \text{ m}^{-2} \text{ day}^{-1}$).

There are also several methods (e.g. Batra et al. 2006; Allen et al. 1998; Bisht et al. 2005) that can provide reliable estimations of area-average R_n using remote sensing information such as land surface temperature, albedo, and atmospheric transmittance.

The sensible heat flux, H , which is the transfer of heat through convection processes in the atmosphere, is conventionally calculated using 1-D flux gradient expression based on a convection analogue to Ohm's Law (e.g. using the Monin-Obukhov formulation, Brutsaert 1982); thus H depends on a turbulent exchange coefficient (h_a), which is a function of wind speed u_a , atmospheric stability and surface roughness. The aerodynamic roughness z_0 , mainly depends on vegetation structure (height and geometry), and z_{0h} , the thermal roughness, depends also on the thermal structure of the canopy and is complex to determine (Kpemlie et al. 2011; Boulet et al. 2012):

$$H = \rho c_p h_a (T_s - T_a) \quad (3)$$

c_p is the specific heat capacity of air ($\text{J kg}^{-1} \text{ K}^{-1}$) and ρ is the density of air (kg m^{-3}).

The ground heat flux, G , which is the transfer of energy from the surface to the soil, depends on thermal characteristics of the soil and time evolution of surface

temperature (Fourier and Heat Storage equations). The estimation of G is still very problematic, and has not been yet addressed in details in the assessment of the performance of the ET-retrieval methods. G can reach high values in arid and semiarid countries. As the other fluxes, ET and H , are obtained from $ET = A \times EF$ and $H = A \times (1 - EF)$, with $A = R_n - G$, the importance to get a suitable parameterisation of both R_n and G is obvious. The problem to get reliable estimates of G is much more complex than R_n , due to the combined effect of soil moisture and land surface properties on this flux.

G is very often parameterized as a constant proportion of R_n , mainly for simplicity sake or for the lack of other possible way to estimate it.

$$G = \frac{1}{k} \cdot R_n \quad (4)$$

Typical recommended values for $1/k$ range from 0.15 to 0.40 in the literature for different types of surface (Choudhury 1987; Humes et al. 1994; Brutsaert 1982; Kustas and Goodrich 1994). Although this approach has been widely applied (Mecikalski et al. 1999; Norman et al. 1995, 2000; Crawford et al. 2000; Deardorff 1978) many studies have shown that the ratio G/R_n is not constant in space or in time and is highly dependent on soil moisture, soil texture and vegetation cover (Clothier et al. 1986; Santanello and Friedl 2003; Fuchs and Hadas 1972; Idso et al. 1975; Cellier et al. 1996; Ogée et al. 2001).

Another commonly used approach using remote sensing is the approximation of $1/k$ as a function of LAI or of a remote sensed vegetation index (Kustas et al. 1993; Moran et al. 1994; Jacobsen 1999; Friedl 2002). In the last years, the parameterisation proposed by Su (2002) using the cover fraction (f_c) as predictive variable was often adopted (e.g., Tang et al. 2010), appearing as a standard empirical method for retrieving G . Although such a formulation allows accounting for the effect of vegetation cover on G , it presents drawbacks in bare or sparse vegetation areas because of the low responsiveness of VIs to changes in soil moisture conditions and to the weak correlation between instantaneous values of G and weekly or biweekly estimates of vegetation indices. These methods using vegetation for parameterising G have been criticized for lacking information on soil thermal properties (Murray and Verhoef 2007a).

An alternative to parameterise G is to consider that G is more closely linked to the sensible heat flux, H , than to R_n . This hypothesis was used since the 70s to estimate G in atmospheric circulation models. Bhumralkar (1975) tested the relationship $G = \gamma H$ (with γ = constant throughout the day = 0.30) and compared its performance with other parameterization schemes. The experimental study of Berkowicz and Prahm (1982)

concluded that G can be considered proportional to H in three contrasted sites, while Cellier et al. (1996) parameterized the ratio G/H as a function of daily mean wind speed. However, Liebethal and Foken (2006) evaluated six parameterisation approaches for G , concluding that H -based relationships do not supply the best performances among the tested approaches.

Prediction of G can be improved by means of analytical or numerical tools based on the resolution of the heat diffusion equation. The tools differ in their needs of local measurements of surface temperature, soil temperature profile, soil moisture, or air temperature (Wang and Bras 1999; Murray and Verhoef 2007a,b; Verhoef et al. 2012; Verhoef 2004; Núñez et al. 2009; Wang and Bou-Zeid 2012). These physically-based methods are universal, but highly demanding in input data and rather complex to handle.

The energy balance equation (Eq. 1, page 14) makes it possible to express LE as a function of sensible heat flux (H), the net radiation (R_n) and the ground heat flux (G) and then from surface temperature:

$$LE = \left(1 - \frac{1}{k}\right) \left((1 - \alpha_s)R_g + \varepsilon_s R_a - \varepsilon_s \sigma T_s^4 \right) - \rho c_p h_a (T_s - T_a) \quad (5)$$

This equation is used for computing latent heat flux in **the residual method**.

Some of the so-called “graphical” RS-based methods such as the triangle method (Jiang and Islam 2001) or S-SEBI (Simplified Surface Energy Balance Index, Roerink et al. 2000) are semi-empirical methods which do not calculate LE as the residual term of the surface balance energy equation, but directly estimate the evaporative fraction (EF) from remotely sensed properties of the surface (LST and NDVI in the case of the triangle method, and LST and albedo in the case of S-SEBI), which is then directly related to EF.

$$EF = f(LST, NDVI \text{ or } albedo) = \frac{LE}{Rn - G} \quad (6)$$

In SVAT models, the latent heat flux is not anymore computed as residual of the energy balance equation (Oliosio et al. 1999). It is fully parameterised from air vapour pressure e_a and a water vapour exchange coefficient (h_s) :

$$LE = \rho c_p h_s (e_s^*(T_s) - e_a) \quad (7)$$

where $e_s^*(T_s)$ is the saturated vapour pressure at the surface temperature T_s . The water vapour exchange coefficient, h_s , depends on the turbulent exchange coefficient h_a , the soil surface resistance to vapour transfer to the atmosphere and the stomatal conductance of the different leaves in the canopy. For its calculation, information on plant structure is required: leaf area index (LAI) and fraction of vegetation cover (f_v). The maximum stomatal conductance ($g_{\max}$), a physiological characteristic of plants, is also required. A parameterisation of stomatal conductance depending on climate and soil moisture (W_i) is usually included in SVAT models. They can solve the energy balance equation resulting in estimation of the different fluxes and surface temperature.

In order to account for the differences in evaporation from the two main types of surface (soil and vegetation), various authors (e.g. Shuttleworth and Wallace 1985; Huntingford et al. 1995; Norman et al. 1995; Van Hurk et al. 1995) have proposed to account separately for the soil surface and the vegetation layer using two energy balance equations (see Olioso et al. 1996, 1999):

$$Rn_v - H_v - LE_v = 0 \quad (8)$$

$$Rn_s - G - H_s - LE_s = 0 \quad (9)$$

with:

$$Rn_v - Rn_s = Rn \quad (10)$$

$$H_v - H_s = H \quad (11)$$

$$LE_v - LE_s = LE \quad (12)$$

In this representation, two surface temperatures – one for the soil and one for the vegetation – have to be estimated independently, for example from thermal measurements in two directions (Norman et al. 1995; Merlin and Chehbouni 2004). This formulation of energy balance is used in the ALEXI model developed by Anderson et al. (1997). Flux calculations follow similar types of equations as in the mono-layer equations.

The required inputs for estimating LE depends on the type of model (see Table 1). It is necessary to define procedures for prescribing these inputs in the models.

Table 1: Input requirements for the different types of model.

Type of model	Meteorological variables	Surface and plant information	Soil information	Others
Residual energy balance equation (Eq. 5)	R_g, R_a, T_a, u_a	$\alpha_s, \varepsilon_s, z_0, z_{0h}, k$		T_s
Graphical methods	R_g, R_a	$\alpha_s, \varepsilon_s, k, (NDVI)$		T_s
SVAT model	R_g, R_a, T_a, u_a	$\alpha_s, \varepsilon_s, f_v, z_0, LAI, g_{max}$	Soil type, W_i	T_s

Meteorological data could be either directly measured *in situ* or obtained from a near meteorological station. The other quantities have to be obtained from remote sensing data, which is the case for surface temperature. Many works have shown that it is possible to derive emissivity (Gillespie et al. 2011; Wan 2008; Jiang et al. 2006), albedo (Román et al. 2009; Cescatti et al. 2012), leaf area index (le Maire et al. 2011; Soudani et al. 2006) and fraction of vegetation cover (Barati et al. 2011; Batra et al. 2006) from remote sensing. Up to now, there is no straightforward ways for estimating W_i from remote sensing data. The parameters z_0 and g_{max} may be estimated from knowledge of the type of canopy and its phenological stage. Difficulties exist for deriving z_{0h} and k .

2.2.2. ET-retrieval methods based on RS information

The first attempts to use RS techniques as a solution for ET-mapping were back in the 70s (eg. Wiegand and Bartholic 1970; Brown and Rosenberg 1973). However, it is not until the 90s that robust methods for continuous ET-mapping have emerged (among others: Norman et al. 1995; Bastiaanssen et al. 1998a,b; Carlson et al. 1995; Roerink et al. 2000; Nishida et al. 2003; Jiang et al. 2004).

In the following we present a classification of the major “historical” models to derive ET from RS data. This classification is not meant to be exhaustive. For a more detailed overview, the reader is referred to Kalma et al. (2008) and Li et al. (2009).

1. *Methods using difference between surface and air temperature*

ET is an endothermic process which takes up heat from the surrounding environment. Therefore, evaporating surfaces will have lower surface temperature than non-evaporating surfaces. The “simplified method” first proposed by Jackson et al. (1977) is based on that principle and calculates the daily ET through the very simple relationship:

$$ET_d = Rn_d^* - B(T_s - T_i)_i \quad (13)$$

where ET_d is daily actual evapotranspiration, Rn_d^* is daily net radiation (mm/day), B is an empirical constant and $(T_s - T_a)_i$ is the difference between soil temperature and air temperature near midday.

Several improved version of the method were proposed (Seguin and Itier 1983; Lagouarde 1991; Seguin 1993), but they all need local calibration.

2. *Surface Energy Balance (SEB) models*

All these methods are based on the Surface Energy Balance equation (Eq. 1 from Chapter 1, section 1.1, page 14).

The residual method calculates the latent heat flux as the residual term of the surface energy balance equation, using equations 1 to 5.

Within the SEB models, we can differentiate the “single-source” (or one-source) SEB models, which recognize the role of surface but do not distinguish between soil evaporation and transpiration, and the “two-source” SEB models in which heat and mass fluxes from the soil and the vegetation are differentiated and allowed to interact.

❖ **One-source models / Spatial variability methods**

The main single-source SEB models using remotely sensed data are methods based on spatial variability of satellite imagery. Evapotranspiration is estimated using spatial variability of:

- Surface temperature and reflectivity (SEBI, SEBS, S-SEBI),
- Surface temperature, reflectivity and vegetation indices (SEBAL, METRIC)
- Surface temperature and vegetation indices (Triangle method, Trapezoidal method)

These methods are based on the contrast between wet and dry pixels which define wet and dry limits to derive ET from the combinations of remotely sensed surface parameters and ground-based measurements. The dry limit (or dry “edge”) is associated with maximum surface temperature and minimum ET, whereas the wet limit corresponds to pixels with lowest surface temperature and highest ET. At the dry edge, the sensible heat flux is equal to the surface available energy: $H = R_n - G$.

(i) *SEBI (Surface Energy Balance Index) and SEBS (Surface Energy Balance System)*

In SEBI, first proposed by Menenti and Choudhury (1993), ET is considered equal to zero at the dry edge (maximum LST) for a given set of boundary layer characteristics (potential temperature, wind speed and humidity). At the wet edge (minimum LST), the surface is assumed to evapotranspire at the potential rate. The potential ET is often calculated by means of the Penman Monteith equation with the internal resistance set to zero. Relative evaporative fraction is obtained by interpolating the observed LST within the minimum-maximum range of LST. Parameterization of the SEBI approach was first proposed by defining theoretical pixel-wise ranges for ET and T_s to account for spatial variability of actual evaporation due to albedo and aerodynamic roughness.

The Surface Energy Balance System (SEBS), detailed by Su (2002) is a more complete, though more complex, version of SEBI. SEBS includes a dynamic model for the thermal roughness and the Bulk Atmospheric Similarity theory for Planetary Boundary Layer (PBL) scaling and the Monin-Obukhov Atmospheric Surface Layer (ASL) similarity for surface layer scaling. A limitation of its use in practice is the high requirement in input parameters that are not easily available.

(ii) *S-SEBI*

The S-SEBI method, developed by Roerink et al. (2000), is based on the albedo-LST space (Figure 1) where three main regions can be distinguished: 1) at low albedo (wet surfaces), surface temperature remains almost unchanged because of high water availability at the surface, this corresponds to area such as open water or irrigated lands; 2) at higher albedo (drier surfaces), surface temperature increases to a certain point with the increase of reflectance (albedo) due to the decrease of ET resulting from lower water availability, which is termed as “evaporation controlled”; 3) after the inflexion, the surface temperature decreases with the increase of surface reflectance (albedo). This stage is called “radiation controlled”.

Figure 1: Theoretical schematic relationship between surface temperature and albedo in The S-SEBI (from Roerink et al., 2000)

(iii) *METRIC and SEBAL*

The main objective of Bastiaanssen et al. (1998a) when developing SEBAL was to retrieve ET estimates with a minimum amount of ground data. The method relies on the estimation of the difference between surface temperature and air temperature dT for each pixel, which can be expressed as a linear expression of dT :

$$dT = a + bT_s \quad (14)$$

a and b are empirical coefficients derived from two points: the driest (hottest) pixel and wettest (coolest) pixel. For the driest pixel, ET is considered equal to zero, and dT_{dry} can be calculated by inverting the single source bulk aerodynamic transfer equation:

$$dT_{dry} = \frac{H_{dry} \times r_a}{\rho c_p} \quad (15)$$

where $H_{dry} = R_n - G$.

For the wettest pixel, $dT_{wet} = 0$ and $ET = R_n - G$. The coefficients a and b can be determined from dT_{dry} and dT_{wet} . The sensible heat flux is then calculated as:

$$H = \frac{\rho c_p dT}{r_a} \quad (16)$$

where ρ = air density (kg m^{-3})

c_p = specific heat of air at constant pressure ($\text{J kg}^{-1} \text{K}^{-1}$)

r_a = aerodynamic resistance to sensible heat transfer between the canopy source/sink height and the bulk air at a reference height above the canopy (s m^{-1}).

This procedure requires wind speed measured at ground to be extrapolated to a height of about 200 m where wind speed at this level is assumed to not be affected by surface variations. H is then corrected for stability through an iterative process using Obukov's length. Figure 2 shows a flow chart of the calculation process in SEBAL. The main problems of SEBAL is that H is highly sensitive to the choice of the dry and wet pixel, and that the model is unreliable when complex topography is involved in the study area.

METRIC developed by Allen et al. (2005, 2007) is similar to SEBAL, but differs in the characterisation of the dry and wet pixels. For the hot pixel, daily surface soil water balance is run to confirm that ET is equal to zero, and for the wet pixel, ET is considered equal to 1.05 ET_r , ET_r being ET for a reference crop (alfalfa) calculated using the standardised ASCE Penman Monteith equation. The wet pixel is chosen in an agricultural area where the vegetation characteristics are similar to the reference crop.

Figure 2: Flow chart of the calculation steps in SEBAL.

(iv) Triangle/Trapezoidal method

The triangle method described by Jiang and Islam (2001) is the one that has been selected in this study to estimate ET from RS data, and is presented in more details in Chapter 3 (section 3.4.). The method involves determining the cold (wet) and hot (dry) edge in the T_s -NDVI space. The evaporative fraction is then calculated using the Priestley Taylor (PT) equation in which the coefficient α is a function of the cold and the hot edge.

❖ **Two-source models***(i) TSM (Two Source Model)*

The TSM developed by Norman et al. (1995) uses the difference between the radiometric surface temperature and the aerodynamic temperature to partition surface fluxes into soil and canopy components (Eq. 8 to 12). Li et al. (2008) used Landsat data at different resolutions, and compared satellite retrievals with ground based flux measurements. The results indicated good agreement at the 30 m and 120 m resolutions, but comparatively poor reproduction of latent heat flux at 960 m resolution, highlighting the issue of sub-pixel scale heterogeneity and the difficulties in assessing remote retrievals at coarse scales.

(ii) Methods using time rate of change in surface temperature with atmospheric boundary models

The analysis of the relationship between the development of the atmospheric boundary layer combined to works on the thermal inertia of land surface (Carlson et al. 1981; Carlson 1986; Brutsaert et al. 1993; Diak and Whipple 1995) led to the development of the TSTIM (Two-Source Time Integrated Model), subsequently named as ALEXI model, presented by Anderson et al. (1997) and Norman (2003). This model is run from measurements in early and mid-morning using thermal infrared data from meteorological geostationary satellites such as GOES and METEOSAT, as well as a knowledge of the initial slope (lapse rate) of the atmospheric temperature profile from synoptic radiosoundings. Mapping at higher spatial resolution (LANDSAT or ASTER) can be achieved using the DisALEXI disaggregation methods (Norman et al. 2003; Anderson et al. 2004; Brunsell and Anderson 2011). A schematic representation of the model is represented in Figure 3.

In ALEXI-DisALEXI, T_a is computed from the description of the morning development of the atmospheric boundary layer, assuming a regional value at a blending height a few dozen meters above the surface.

Figure 3: From Norman et al. (2003). Schematic diagram representing the coupled ALEXI–DisALEXI modeling scheme, highlighting fluxes of sensible heat (H) from the soil and canopy (subscripts “c” and “s”) along gradients in temperature (T) and regulated by transport resistances R_a (aerodynamic), R_x (bulk leaf boundary layer), and R_s (soil surface boundary layer). DisALEXI uses the air temperature predicted by ALEXI at 50 m AGL (T_a) to disaggregate 5-km ALEXI fluxes, given vegetation cover [$f(\phi)$] and directional surface radiometric temperature [$T_{RAD}(\phi)$] information derived from high-resolution remote sensing imagery. See Norman et al. (2003) for further details

3. Methods using surface temperatures and meteorological data

(i) Crop water stress and water deficit indices CWSI, WDI

The CWSI (Crop Water Stress Index, Moran et al. 1994; Idso et al. 1981; Jackson et al. 1981) and the WDI (Water Deficit Index, Moran et al. 1994) are indexes derived from the trapezoidal method, similar to the triangle method, and ET is calculated in comparable ways. The main difference lies in that for the trapezoidal space, as opposed to the triangle space, there is no need to have a full range of pixels representing wet/dry/vegetated/non-vegetated surface, because the four vertices of the trapezoid are defined using ground-data.

(ii) Normalized Difference Temperature Index NDTI

Methods such as SEBAL, S-SEBI and the triangle method are limited by the fact that each condition, i.e. very wet and very dry, fully vegetated and completely bare surfaces is not always present on a given image. McVicar and Jupp (2002) developed the Normalised Difference Temperature Index (NDTI) to overcome this limitation. NDTI defines the temperatures for very dry and very wet conditions by inverting a two-source

SEB model and places the observed T_s values in an envelope defined by the modelled maximum and minimum temperatures.

(iii) Methods based on the complementary relationship

The complementary relationship (CR) first proposed by Bouchet (1963), later revised by Morton (1983) and Granger (1989) states that, as the land surface dries, the decrease in actual ET is accompanied by an increase in the potential ET. This is expressed as (Granger 1989):

$$E_p + \left(\frac{\gamma}{\Delta}\right) E_a = \left(\frac{\Delta + \gamma}{\Delta}\right) E_w \quad (17)$$

where E_p is the potential evaporation that would occur under prevailing atmospheric and energy conditions if evaporation was not water limited, E_a is the actual evaporation and E_w is the evaporation of an extended wet surface when $E_a = E_p = E_w$, Δ is the slope of saturated vapour pressure at air temperature and γ is the psychrometric constant. E_p can be estimated by the Penman-FAO (1977) equation (Brutsaert and Stricker 1979) and E_w is computed using the Priestley-Taylor equation (Priestley and Taylor 1972). In their study over the Southern Great Plains, Venturini et al. (2008) used the 1 km MOD11 product as the source of surface temperature data and obtained air and dew point temperature profiles from MOD07. Their results indicate that E_a may be obtained with an estimation error of $\pm 15\%$ when compared with flux measurements obtained at 15 EBBR (Energy Balance Bowen Ratio) stations.

2.2.3. Advantages and limitations of RS-based ET-retrieval methods

The main advantages are:

- Limited requirements in ground-based input data
- Relatively simple to apply
- Requires reasonable computational capacity

The main limitations are:

- Discontinuity of the RS-data which depends on the overpass frequency. In particular, LST, a basic input, is not available on cloudy days. A way to overcome this problem is the use of gap filling procedures such as described by Anderson et al. (2007a,b). Jiang et al. (2009) developed a space-time interpolation algorithm which uses information on cloud free days to fill the cloudy pixels on partly cloudy days, and to interpolate temporally to fill the gaps. By this way, they managed to generate a full daily ET time series of 730 days over South Florida for 1998 and 1999 with reasonable bias and RMSE. A complementary solution is the use of coupling models based on TIR remote sensing with data obtained with passive microwave sensors which have lower spatial resolution but are not affected by clouds (Renzullo et al. 2008; Kalma et al. 2008).
- ET retrieved, measured at overpass time, is an instantaneous value. This aspect has been addressed by many authors, who proposed different methods to convert instantaneous ET values to daily estimates. A common approach is to use a weighting technique based on the similarity between the diurnal course of ET and that of other components of the surface energy balance (Brutsaert and Sugita 1992). Jackson et al. (1983) assumed that the diurnal course of ET would generally follow the course of solar radiation throughout the daylight period, whereas Seguin and Itier (1983) and Sanchez et al. (2008) considered the net radiation. Another approach is the approximation of the diurnal course of ET to a sine function (Boegh et al. 1999; Batra et al. 2006; Li et al. 2009). An alternative solution, quite widely accepted, and easily applicable in the case of the triangle method, is based on the observation (Crago 1996; Caparrini et al. 2004) that evaporative fraction remains fairly constant for most of the day-light hours. Hence, with EF estimated with the triangle method, the instantaneous ET could be scaled up to daily values if R_n is known over 24 hours, with the assumption that G is negligible over the diurnal cycle (Kalma et al. 2008; Jiang et al. 2009; Li et al. 2009). Other approaches are the use of the ratio ET to potential ET (Colaizzi et al. 2005; Gentile et al. 2007; Hoedjes et al. 2008; Chávez et al. 2008), the diurnal evolution of the albedo (Jacob and Olioso 2005), and the conduction flux into

the soil and the net radiation (Santanello and Friedl 2003; Kpemlie et al. 2011). In the METRIC algorithm, Allen et al. (2007) proposed a constant reference ET fraction ($ET/ET_{reference}$), which is believed to better capture the effect of advection and changing wind and humidity condition during the day. Errors between 5% and 25% in extrapolating ET from instantaneous to daily values were reported (Chávez et al. 2008; Colaizzi et al. 2005).

- Compromise necessary between spatial/temporal/spectral resolutions. On the one hand, systems such as AVHRR, MSG, and MODIS provide daily observations with low (e.g. kilometric) spatial resolution. On the other hand, systems such as Landsat or ASTER provide high spatial resolution with poor revisit capabilities of about two weeks. Over land surfaces, several attempts have been made to disaggregate low resolution imagery down to a few tens of meters (Agam et al. 2007; Inamdar et al. 2008; Inamdar and French 2009; Merlin et al. 2010), with the aim of exploiting the daily revisit of AVHRR, MODIS or Meteosat systems, making it possible the monitoring of rapid changes in relation with rainfall for instance. But despite some progress, the results are not robust enough, partly because it is difficult to account for the variability of the various fields within the coarse resolution pixels. In particular, fields covered with the same crop may display important differences in water status and evapotranspiration rates, in relation to irrigation or soil hydrodynamic properties. The validity of the calculation of evapotranspiration at the scale of kilometric pixels, in general heterogeneous while the equations are theoretically valid only for homogeneous surfaces, has been relatively little investigated. Moran et al. (1997), Bouguerzaz et al. (1999), Kustas et al. (2004), Li et al. (2008) showed that spatial heterogeneity can have substantial impacts on ET estimates at the kilometer resolution.
- Problem of accuracy in LST. Kpemlie (2009) showed that an acceptable accuracy, between 10 and 15%, on latent heat flux estimation using the residual surface energy balance equation requires accuracy around 0.5 K in surface temperature. This requirement cannot be met in practice with current remote sensing systems (Jacob et al. 2008), since difficulties in sensor calibration, poor knowledge in surface emissivity and atmospheric effects strongly affect surface temperature estimates.
- Uncertainties in thermal and aerodynamic roughness length can lead to large errors (Wassenaar et al. 2002). Hasager et al. (2003) showed that surface aerodynamic properties (in particular the thermal roughness) were the most important parameters to consider in the process of aggregation over heterogeneous areas. The other input data have generally a much more linear behavior (albedo, emissivity, surface

temperature). The storage of heat in the soil is also problematic in many situations and can generate large errors in ET estimates, in particular for partial canopy cover (Carlson et al. 1995; Santanello and Friedl 2003; Matsushima 2005; Murray and Verhoef 2007a,b; Anderson et al. 2007a,b; Kpemlie 2009; Boulet et al. 2012). The accuracy of meteorological data used to drive estimation of ET has also a strong impact, in particular when considering the spatial variations of air temperature (Timmermans et al. 2008).

2.3.ET estimation by means of Land Surface Models (LSM)

2.3.1. Role of LSMs

LSMs or SVAT models include a detailed description of the processes regulating evapotranspiration alongside with other biophysical processes taking place at the land surface. In these models, energy balance equations are fully solved providing surface temperature as a solution of the set of equations. Conversely to semiempirical approaches, LSMs give access to a detailed description of soil and vegetation canopy processes, and not only to a limited number of final variables such as evapotranspiration. They simulate intermediary variables linked to hydrological or physiological processes (Oliosio et al. 1999).

LSMs have been mostly designed as surface parameterisations of atmospheric global circulation models (AGCM) in order to account for the mass and energy exchanges that occur between the Earth surface and the atmosphere above, and also to account for runoff coming from land surface hydrology to the oceans in oceanic global circulation models (OGCM) (e.g. Dickinson et al. 1986; Sellers et al. 1996; Noilhan and Planton 1989) (Figure 4).

Figure 4: Role of Land Surface Models. Relationship with AGCMs and OGCMs.

The main modules of a LSM are (Figure 5):

- a part dealing with surface energy exchanges with the atmosphere,
- hydrology module that solves the water cycle
- carbon cycle module

The new generation LSMs tend to increase in complexity and to include modules incorporating other processes such as the nitrogen cycle or vegetation dynamics, among others.

Figure 5: Main “ingredients” of a LSM. From Bonan (2008).

2.3.2. Parameterisation of different processes

LSMs rely on the parameterisation of the main following processes:

- radiative transfer, often following a simple Beer–Lambert law or using radiative transfer schemes as in Hope et al. (1988), or Camillo (1991);
- turbulent transfer, generally based on the resistive schemes by Deardorff (1978), Choudhury (1989), or van de Griend and van Boxel (1989);
- heat and water transfer in the soil; in most models, a system with two soil reservoirs is used, one representing the root zone and the other one the first centimeters of the soil which are directly concerned by soil evaporation (e.g., Deardorff 1978; Carlson et al. 1990);
- water transfer from the vegetation cover to the atmosphere, based on an adequate description of stomatal regulation and water extraction by the roots; the stomatal conductance may be either, directly related to the soil water content (Taconet et al. 1986; Noilhan and Planton 1989), or indirectly using a description of water transfer from the soil to the leaves along water potential gradients (Lynn and Carlson 1990; Braud et al. 1995; Olioso et al. 1996);

- Presently, most LSMs also incorporate photosynthesis parameterisation that account for stomatal regulation or water status of leaves (Zur and Jones 1981; Oliso et al. 1996; Sellers et al. 1996; Carlson and Bunce 1996).

LSMs usually require information on vegetation structure (LAI, height), optical properties of soil and vegetation, physiological properties of vegetation (stomatal conductance description, water transfer from soil to plants), thermal and hydraulic properties of the soil, and atmospheric conditions (air temperature and humidity, wind speed, incident short and long wave radiation).

The representation of the soil–vegetation–atmosphere system description varies considerably in complexity, from simple one-layer models (Figure 6), which only describe global exchange of the soil–vegetation system with the atmosphere, such as evapotranspiration (Soer 1980; Courault et al. 1996), to detailed models that describe microclimate profiles inside the canopy and/or the soil (Norman 1979; Meyers and Paw U 1987; van de Griend and van Boxel 1989; Bruckler and Witono 1989; Braud et al. 1995).

Presently, intermediate-complexity coupled soil-vegetation models are generally used (Figure 7). They partition energy fluxes into fluxes originating from a single vegetation layer and from the soil surface (Taconet et al. 1986; Lynn and Carlson 1990; Camillo 1991). Such models are less complex to handle than multilayer models, but they allow simulating separately vegetation transpiration and soil evaporation, which behave in different ways depending on environmental conditions. Because of the growing interest in simulating the carbon cycle in global change studies, many of these models have been extended to the simulation of photosynthesis (Carlson and Bunce 1996; Sellers et al. 1996).

Figure 6: From Olioso (1999) (adapted from Raupach and Finnigan 1988). Schematic structure of single-layer and multilayer SVAT models. Symbols: g_{vi} : surface conductance of vegetation layer i ; H : sensible heat flux; H_s : sensible heat flux from the soil surface; H_{vi} : sensible heat flux from vegetation layer i ; h_{vi} : turbulent exchange coefficient for vegetation layer i ; LE : latent heat flux; LE_s : latent heat flux from the soil surface; LE_{vi} : latent heat flux from vegetation layer i ; q_a : air humidity; q_{aci} : air humidity inside vegetation layer i ; r^* : surface resistance; r_a : aerodynamic resistance; R_g : global solar radiation; T_a : air temperature; T_{aci} : air temperature inside vegetation layer i .

Figure 7: From Olioso (1999). Schematic structure of a two-layer SVAT model. Symbols: g_s : surface conductance of the soil; g_v : surface conductance of the vegetation layer; H : sensible heat flux; H_s : sensible heat flux from the soil surface; H_v : sensible heat flux from the vegetation layer; h : turbulent exchange coefficient between the canopy and the atmosphere; h_s : turbulent exchange coefficient between the soil surface and the air inside the canopy; h_v : turbulent exchange coefficient between the vegetation and the air inside the canopy; LE : latent heat flux; LE_s : latent heat flux from the soil surface; LE_v : latent heat flux from the vegetation layer; q_a : air humidity; q_{ac} : air humidity inside the canopy; R_g : global solar radiation; T_a : air temperature; T_{ac} : air temperature inside the canopy.

2.3.3. Evolution of LSMs

❖ First generation LSMs

In the 70s, the first LSMs were very simple, using basic versions of the energy balance equation. There was no explicit treatment of vegetation, and surface resistance did not include canopy resistance. Aerodynamic resistance for heat, water and momentum were considered equal, and only one single layer was contemplated for soil moisture. Heat conduction into the soil was not taken into account, and no seasonal or diurnal cycle was considered. The soil had fixed properties and a constant depth. The hydrological processes were computed following the simple “bucket” approach proposed by Manabe (1969) in which evaporation is limited by soil water content below a threshold, and if the moisture exceeded that prescribed limit, further precipitation would generate runoff (saturation excess runoff). The Project for Intercomparison of Landsurface Parameterisation Schemes (PILPS) has shown that the model was inadequate for diurnal to multi-annual scale surface hydrology representation (Qu et al. 1998; Wood et al. 1998).

Deardroff (1978) introduced a method for simulating soil temperature and moisture in two layers and vegetation as a single bulk layer that shielded a fraction of the ground from solar radiation. This approach was revolutionary for the land surface modelling community (Pitman 2003), since processes were treated explicitly and mathematically for the first time.

❖ Second generation LSMs

In the 80s, the second generation LSMs incorporated several improvements in comparison to the 1st generation LSMs. The main changes were:

- Following the advances brought by Deardroff (1978), differentiation between soil and vegetation at the surface are universally adopted. Albedo can vary spatially across a grid square, as well as varying depending on the wavelength of the incoming solar radiation (PAR vs. NIR).
- Explicit biophysical controls on evaporation are included. Photosynthesis and stomatal conductance are taken into account. In particular, stomatal response depends on PAR, humidity and temperature (empirical modelling of stomatal conductance). The “big-leaf” approach is used to scale up fluxes exchanges from leaf

to canopy, assuming that the canopy has the same relative response to the environment as any single leaf. Canopy resistance can be calculated from the stomatal conductance or resistance via appropriate scaling, and from water potential. The latter is related to soil water content in the root zone, root distribution and evaporative demand. Therefore, the fluxes of water from the soil and from intercepted precipitation on canopy are represented separately, having distinct aerodynamic resistance and canopy-related resistance.

- The models are able to represent explicitly the impact of vegetation on momentum transfer, and on water and energy budget. They account for canopy roughness and its effects on turbulence exchange of heat and mass between the surface and the atmosphere.
- Multi-layer hydrology is also incorporated to these 2nd generation LSMs to simulate the water cycle. Some examples are the Biosphere Atmosphere Transfer Scheme BATS (Dickinson 1984) and the Simple Biosphere Model SiB (Sellers et al. 1986). Several layers are considered into the soil, and the water transfer in the soil is modelled using soil type specific formulae based on Richards equation, or soil physics formulae proposed by Philip (1957) and Hillel (1982). Vertical transfer of water within the soil profile uses a set of diffusion equations based on Darcy's law. Hydraulic conductivity and soil moisture potential are assumed soil moisture dependent. This increase in complexity is accompanied by the need of an increasing number of input parameters such as saturated hydraulic conductivity or soil moisture potential at saturation, among others. Several approaches to parameterise runoff with different level of complexity are considered.
- A great effort is also invested to parameterise snow melting. This aspect is not described here, since this PhD focuses on semi-arid regions.

As shown in PILPS Project, these models outperform those of first generation. The modelling of surface atmosphere interactions on the time-scale of days, precipitation weather forecast and European soil temperature prediction are all improved (Beljaars et al. 1996; Viterbo et al. 1999).

❖ **Third generation LSMs**

In the 90s, substantial improvements were made in the representation of plant physiology and the carbon cycle was included in LSMs. Empirical representations of vegetation conductance are replaced by semi-empirical approaches that better describe

the physiological processes taking place. In the carbon cycle modelling, the leaf assimilation of carbon is limited by the efficiency of the photosynthetic enzyme system (Rubisco-limitation), the amount of PAR captured by the leaf chlorophyll and the capacity of the leaf to utilize the products of photosynthesis.

Multi-layers approach gives a better scaling up method than the “big-leaf” approach to go from leaf-models to canopy-scale models, giving estimates of canopy resistance, canopy photosynthesis and canopy respiration. The models are more accurate in predicting net carbon assimilation and net primary productivity.

Therefore, the third generation LSMs represent a fundamental advance towards a realistic representation of the degree of coupling between the surface and the atmosphere and the different feedback loops that control the surface fluxes. Some examples of third generation LSMs are SiB2 (Sellers et al. 1992), LSM (Bonan 1995; Collatz et al. 1991) and MOSES, the predecessor of JULES (Cox et al. 1999).

❖ **Current LSMs**

More recently, LSMs started to include long term response of ecosystems dynamics to climate change. This is achieved by merging traditional LSMs with ecological models, such as TRIFFID (Top-down Representation of Interactive Foliage and Flora Including Dynamics) in JULES (Cox 2001). Another example is IBIS (Foley et al. 1996). Such LSMs are called “biogeochemical” because the land surface parameterisation accounts for the geophysics, biogeochemistry and biogeography of terrestrial ecosystems. They require a multidisciplinary approach, involving the collaboration of different scientific communities (hydrologist, land surface modellers, ecologists, etc.).

2.3.4. Advantages and limitations of LSMs

The main advantages are:

- Detailed description of a large number of soil and vegetation canopy processes, and not only of a limited number of final variables such as latent (LE) and sensible (H) heat fluxes or net primary production (e.g. Sellers et al. 1996).
- Because the processes are described in a comprehensive and mechanistic way, LSMs are universally valid and could be applied to any place.
- They could be run at short time-step and continuously, in satisfactory agreement with the timescale of the physical processes being simulated.

The main limitations are:

- High complexity. The degree of realism of a LSM generally depends on their structural complexity (i.e. the detail in the model physics), the representativeness and configuration of the different components (such as the number of soil layers), the quality of the input data used for parameterisation. Complexity can be substantially increased when the parameterisations account for detailed site-specific conditions such as local climate, biophysical and geophysical characteristics (Moran et al. 2004).
- Numerous input parameters required. The reliability of complex models over large areas is limited by our ability to provide them with the required input variables and parameters concerning atmospheric, soil and plant characteristics (such as soil moisture, soil hydrodynamical properties, aerodynamic roughness, leaf area index, etc.). The lack of accurate knowledge of those parameters leads to high levels of uncertainty (Cayrol et al. 2000).
- No representation of horizontal transport. Since these models are generally one-dimensional vertical representations, they have little or no representation of horizontal transport and are limited in their capacity to produce spatially distributed outputs (Petropoulos et al. 2009).

2.4.Data assimilation

2.4.1. Description

Data assimilation has been firstly used by meteorologists to construct daily weather maps, displaying variations of environmental variables such as pressure and wind speed over space and time (McLaughlin 1995). Data assimilation technique can be defined as the process in which all available information is used in order to estimate objective variables as accurately as possible (Talagrand 1997; Bouttier and Courtier 1999). Many existing assimilation algorithms can be considered as approximates of statistical linear estimation (Rabier et al. 1993). Data assimilation schemes are statistical optimisation-techniques that minimize the errors in estimates derived from merging noisy observations and uncertainty of models in a statistical sense. Selection of a data assimilation technique should be based on a compromise between making the best use of all available information (optimality) and computational efficiency, flexibility, and robustness. Such a compromise should account for the specific goals of the study because evaluation criteria could conflict (Margulis et al. 2002).

There are two basic approaches to data assimilation: sequential assimilation (e.g., Ensemble Kalman Filter and optimal interpolation), that only considers observations made in the past until the time of analysis, which is the case of real-time assimilation systems (Crow and Kustas 2005; Caparrini et al. 2004; Margulis et al. 2005; Reichle et al. 2002a,b; Anderson 2001; Huang et al. 2008), and non-sequential, or retrospective assimilation (e.g., 4-dimensional variational assimilation), where observations from a period posterior to the study period can be used, for instance in a reanalysis exercise (Courtier et al. 1998; Županski and Mesinger 1995; Margulis and Entekhabi 2003b; Seo et al. 2003; Caparrini and Castelli 2004).

Another distinction can be made between methods that are intermittent or continuous in time. In an intermittent method, observations can be processed in small batches, which is usually technically convenient. In a continuous method, observation batches over longer periods are considered, and the correction to the analysed state is smoothed in time, which is physically more realistic. The combination of the two classifications gives a total of four basic strategies for data assimilation, which are represented in Figure 8.

Figure 8: From Bouttier and Courtier (1999). Representation of four basic strategies for data assimilation, as a function of time. The way the time distribution of observations ("obs") is processed to produce a time sequence of assimilated states (the lower curve in each panel) can be sequential and/or continuous.

LSMs can be improved by means of assimilating of RS-data broadly in two ways:

Calibration

Monte Carlo (MC) simulations using RS-data is an usual option to calibrate input parameters or define initial states of LSMs. The MC method consists in repeating random sampling of input parameters in order to solve a mathematical or physical system. The set

of input parameters that minimises the difference between the solution given by the LSM and remote sensing data is then identified (Arai 2008).

Other iterative optimization techniques such as the Newton's method or Quasi-Newton algorithms are alternative statistical approaches for finding the minimum (Dorigo et al. 2007). These methods are computationally intensive which makes its application for operational use difficult in many cases (Liang 2004).

Another way of calibrating LSMs using RS data is using the Adjoint-to-the-model. In this method, an objective ("cost") function, J , is identified (for example, the weighted error when comparing observed RS measures with estimated values from the model), and is minimised. This is done evaluating the "cost" function through a forward integration, and subsequently, a "backward" integration of the adjoint model returns the gradient, or sensitivity, of the cost function, $\delta J / \delta X$, with respect to a given set of control variables, X . Figure 9 shows a conceptual diagram of an adjoint model. The development of the adjoint model implies an important programming effort, but once it is working and validated, it usually requires much less computational time than using the MC method or another calibration scheme.

Figure 9: Conceptual diagram of the Adjoint of a model.

The above mentioned methods require an initial guess of the solution. The correctness of this initial guess can be critical to get a successful optimization. Otherwise the solution could be trapped in a local minimum (Qiu et al. 1998). Furthermore, the accuracy of the solution depends on an appropriate choice of the cost function.

Correcting the model when observation is available

Rather than retrieving model parameters or initial conditions, the model parameters can be fitted by comparing the model outputs to remote sensing observations each time they are available (François et al. 2001; Reichle et al. 2002a; Pipunic et al. 2008).

In these data assimilation techniques, the observed information is accumulated into the model state by taking advantage of consistency constraints with laws of time evolution and physical properties (Bouttier & Courtier, 1999). They have been widely developed in meteorological applications, for instance by introducing observations in atmospheric models used for numerical weather prediction (Talagrand & Courtier, 1987). Different methodologies and mathematic tools, such as Kalman filters (Kalman 1960), have been developed for implementing assimilation procedures.

Several authors have attempted to use data assimilation techniques combined with a numerical model to estimate regional surface turbulent heat fluxes (Boni et al. 2001; Crow and Kustas 2005; Caparrini et al. 2004; Margulis et al. 2005; Pipunic et al. 2008). Boni et al. (2001) developed a land data assimilation system to estimate latent heat flux and surface control on evaporation with the dynamic equations for surface temperature as the constraint. Caparrini et al. (2003) proposed a land data assimilation scheme with sequences of multi-satellite remotely sensed surface temperature measurements and data from surface micrometeorological stations to estimate the surface energy balance components in a basin with varying surface conditions. Margulis et al. (2005) compared the VI- T_s triangle method to a variational data assimilation method for estimating surface turbulent fluxes from radiometric surface temperature observations, and their results have shown that the assimilation approach performs slightly better than the triangle method.

2.4.2. Advantages and limitations of data assimilation techniques

Data assimilation techniques offer the advantages of both LSMs and RS-based models:

- Horizontal and vertical coverage. The combined use of LSMs with remote sensing data allows merging of the horizontal coverage, repetitive nature and high spatial detail of satellite remote sensing with the vertical coverage and temporal continuity of the LSMs.
- Assimilation procedure estimates not only latent heat flux but also the other intermediate variables related to the turbulent heat fluxes.
- The data assimilation procedure can produce estimates at a much finer resolution.
- Data assimilation scheme can merge spatially distributed information obtained from several data sources with different resolutions, coverage, and uncertainties (Margulis et al., 2002).

The main limitations are:

- Assimilation schemes are relatively more computationally demanding than the remote sensing ET models.
- In most practical cases the problem is ill-defined because data are scarce and only indirectly related to the model variables.
- The problem is generally of a highly nonlinear nature and the true algebraic solution does not exist. Hence, linear data assimilation techniques (Kalman filter) are not adequate, and more complex solutions have to be considered (Ensemble Kalman filter, Unscented Kalman filter, Sampling importance resampling particle filter, unscented particle filter, see Han and Li 2008 for a review), with robust approximate iterative solutions to solve the problem.

2.5. Conclusion

Areal estimation of ET is needed for a wide range of applications such as (a) irrigation management and crop water demand assessment, (b) plant growth, carbon and nutrient cycling and production modelling in dry land agriculture and forestry, (c) catchment hydrology, and (d) larger scale meteorology and climatology applications (Kalma et al. 2008). The main methods to retrieve information about spatial and temporal values of ET are either remote sensing based methods, or Land Surface Models, or a combination of both through data assimilation techniques.

In agriculture and irrigation management, high spatial and temporal resolution is needed, and therefore the use of remote sensing techniques is limited by the spatial and temporal resolution of the satellite sensors. For most of the practical applications in those fields, the 2-weeks revisiting frequency of high resolution sensors platforms (Landsat, ASTER) represents a strong limitation. In the future, the application of RS-techniques will rely on enhancing the temporal resolution of high-spatial resolution sensors, together with the development of improved methods for temporal extrapolation and spatial disaggregation techniques. For larger scale applications such as catchment hydrology or climatology and meteorology, the 1 km resolution daily data from MODIS or AVHRR is satisfactory.

Land surface models as an alternative technique to retrieve spatial distribution of surface fluxes have the great advantage of including a mathematical description of the biophysical processes taking place, increasing the understanding of the underlying processes. However, their application is highly limited in practice by the impossibility to provide the model with accurate values for the input parameters. Combining LSMs with remote sensing data through data assimilation techniques is a promising way of overcoming this problem, and would allow the merging of the temporal continuity of LSMs with the spatial coverage and accuracy of remote sensing methods. However, the complexity of these methods and their computational requirements restrict its spread as a generalised tool within the scientific community, and currently, those techniques are only routinely used in meteorological forecasting.

Chapter 3: Material and Methods

3.1. Introduction

The data used in this PhD work presents a wide variety both in their nature and in their geographical origin. Regarding the kind of data, three types can be distinguished: meteorological data, surface-flux data and satellite data. With respect to the provenance of the data, the common feature is that they concern semi-arid countries. The two main geographical areas are:

- the AMMA sites in South-West Africa comprise 4 study sites (two in Mali, one in Benin and one in Niger). Data collected at these sites were used (i) in Chapter 4, for the development of the new parameterisation of G (ii) in Chapter 6, for the analysis of spatiotemporal evolution of ET in Sahelian regions.
- The River Segura Basin (RSB), in South-East Spain. RS-data collected over RSB was studied in Chapter 5, where we compare a LSM with an ET-retrieval algorithm. In Chapter 6, we present (i) the climatology of surface fluxes based on a 12-year time series corresponding to three SRB inland sites equipped with ground weather stations (Calasparra, Jumilla and Murcia), and (ii) the water balance of the Mar Menor lagoon, located in coastal part of RSB.

This chapter first describes the different sites, with the respective ground meteorological data collected at each site (Section 3.2.). In section 3.3., the satellite data and MODIS are detailed. Section 3.4. presents the selected RS-based algorithm to retrieve ET. The Chapter ends with a general description of the main modules of LSM JULES (Section 3.5.).

3.2. Ground data

3.2.1. AMMA sites

- *Site description*

The data were collected at observation sites managed by AMMA (African Monsoon Multidisciplinary Analysis) partners within the AMMA Catch observation system (Lebel et al. 2009). Information on AMMA project can be found at <http://amma-international.org/>. One of the main objectives of AMMA was to improve the knowledge and understanding of the West African monsoon and its variability with an emphasis on daily-to-interannual timescale. Figure 10 shows the location of the sites used in this study, which have contributed ground truth to previous analyses of remote sensing data (Kergoat et al. 2011). The ground data used in this study included mainly net radiation, sensible heat flux, soil moisture at two depths and rainfall.

Eguerit and Kelma sites (Mali)

Mean annual rainfall over these two sites is around 370 mm, occurring from June to September with no rain at all from October to April (Frappart et al. 2009). The landscape is dominated by grasslands growing on sandy dunes. Bare soil is also widely present in the area, either with rocks topped with gravels or loamy shallow soil, and the rest consists of valleys and low-lands with clay soil (Timouk et al. 2009). The Eguerit site is located on a rocky surface, whereas the Kelma site lies on a clay soil, covered by acacia forest (De Rosnay et al. 2009). The clay soil presents a low permeability to water, and the consequence of this feature is that Kelma site gets completely flooded during the wet season.

Banizoumbou site (Niger)

The studied area is located in the cultivated Sahelian environment of southwest Niger. The climate is semiarid with a potential evapotranspiration near 2500 mm yr⁻¹ and a yearly mean rainfall of 570 mm. At the seasonal scale, 90% of the annual rainfall, mostly of convective origin, occurs during June to September. The natural vegetation is mainly woody savannah (dominant species: *Acacia* sp., *Balanites aegyptiaca*, *Prosopis* sp.) but under increasing land clearance most of the sandy slopes are now covered by a patchwork of fallow (dominated by *Guiera senegalensis*) and rain-fed millet fields. On the plateaus, the vegetation consists of the typically semi-arid banded vegetation pattern of “tiger bush” (*Combretum micranthum*, *Combretum nigricans*, *Combretum glutinosum*, *Guiera*

senegalensis). In the more clayey valley bottoms, the original bushy vegetation (*Piliostigma reticulatum*, *Bauhinia rufescens*, *Acacia* sp.) has now almost disappeared for cultivation of some specific water-demanding domestic crops (cassava, groundnut or sorghum) (LeBlanc et al. 2008). The flux station is located in a millet field (Cappelaere et al. 2009).

Figure 10: Location of the flux sites. Coordinates : Eguerit Lon -1° 23' 24" Lat 15° 30' 0". Kelma Lon -1° 34' 12" Lat 15° 13' 12". Banizoumbou: Lon 2° 37' 48" Lat 13° 31' 12". Bellefongou: Lon 1° 43' 12" Lat 9° 47' 24".

Bellefongou site (Benin)

Over this site, annual rainfall is 1200 mm, with 60% of the annual rainfall concentrated between July and September. The wet season extends from April to October. However, isolated rainfall can occur throughout the year, with the lowest probability during December and January. Natural vegetation is composed of a patchwork of dry forests and savannah, with dense and tall herbaceous strata, mainly composed of perennial grasses, and more or less dense woody strata. The original landscape has been modified by increasing cropping practices (Seghieri et al. 2009). The flux station is set over a clear forest. Trees are more than 10m high and less than 15m. They keep their leaves during the entire year except 2 months in December and January, but all species are not in phase. The surface characteristics are from loamy sand to sandy loam. An herbaceous strata grows between trees, being more dense where trees are more sparse. This forest site is quite different from the acacia forest of the Kelma site which is flooded during the wet season.

- ***Meteorological data***

Net radiation data

All the sites were equipped with identical sensors to monitor the components of the net radiation at the surface (4-component sensor Kipp&Zonen CNR1 Radiation), except for the Bellefoungou site for which a NR-Lite sensor (for net long wave radiation) and two Skye pyranometers (for upward and downward solar radiation) were installed at 5m high. The albedo values used in this study were calculated from the ratio of the reflected to incident shortwave radiation provided by the sensors. The station was installed in an open area and the estimated albedo was not affected by shading except in the early morning and late afternoon.

- ***Flux data***

The sensible turbulent flux was measured by means of the eddy-covariance (EC) technique. The flux stations consisted of a three dimensional sonic anemometer (Model R3-50, Gill Solent Instruments, Lymington, UK) which provided measurements of the fluctuations of vertical velocity and air temperature. The sonic anemometer was controlled by a specially designed solid state logger (Center for Environment and Hydrology, Wallingford, UK) which recorded the 20 Hz raw data and the 30-minute averages of fluxes. More details of the complete installations and data processing can be found in Mougin et al. (2009) for Eguerit and Kelma, in Ramier et al. (2009) for Banizoumbou and at the AMMA-CATCH website:

http://www.lthe.fr/catch/observation/measurement_doc/EF9_AE.H2OFlux_Odc_en.pdf for Bellefoungou. A detailed description of surface flux measurements for all sites can also be found in Lloyd and Taylor (2005).

3.2.2. Segura River Basin sites

The Segura River Basin, located in southeast Spain, covers an area of 18,870 km², representing 3.7% of the Spanish territory. The basin is shared by several Spanish provinces: Murcia (11,126 km²), Albacete (4,765 km²), Alicante (1,082 km²), Almeria (907 km²), Jaen (646 km²) and Granada (80 km²).

The highest topographic features of the basin are the Cazorla Mountains with Mount las Banderillas (1,982m), the Segura Mountains with Mount las Cibras (2,081m), the Taibilla Mountains with Mount Los Odras (1,887m), the Alcaraz Mountains with Mount Padrastró (1,502m), the Calar del Mundo Mountains with Mount Argel (1,692m), and the Espuña Mountains with Mount Miamón (1,761m).

Eighty percent of the basin extension belongs to the Segura river (14,936 km²), 1,103 km² corresponds to closed basins situated between the river Segura Basin and the river Júcar Basin, and the rest is composed by small watercourses characterised by low average baseflow, very irregular in time, with quick level rise and long periods of almost completely dried state. Some examples of those ephemeral channels are: río Nacimiento, río Seco, Rambla del Albuñón, Rambla de Benipla and Rambla de Mazarrón.

All the features that determine the climate of the basin (latitude, climatic atmospheric factors, topography, orientation and exposure, and distance to the coast) result in a wide array and diversity of conditions (Grindlay et al. 2011). As a consequence the whole territory of the Segura River Basin presents great climatic contrasts, frequent droughts, torrential rains, recurrent floods, high temperatures and heavy frosts (Romero Díaz et al. 1992). Significant climatic differences are observed; from one face of a mountainous slope to another, from the highlands to the littoral fringe, or from one geographical area to another; on occasions there are local variations directly related to topographic factors that give origin to local eco-climates.

Figure 11: Location map of the Segura river basin, main rivers and the three study sites

The interior part of the basin has a continental climate, with average annual temperatures of 10 to 12 °C with high fluctuations. Rainfall varies from 400 to 1,000 mm with a fairly even distribution throughout the year, with relative maximums in spring and autumn. The coastal area is characterised by mean yearly temperatures of around 17 to 18°C and rainfall from 200 to 350 mm with maximums in spring and autumn, which defines the typical Mediterranean climate.

The south-east part of the basin is especially arid (Vidal-Abarca et al. 1992; Garcia-Latorre et al. 2001; Thornes and Rowntree 2006), with important problems of

erosion and desertification (Onate and Peco 2005), associated in turn with an inadequate and unsustainable treatment of water and soil in the agricultural terrains (Martínez-Fernández and Esteve-Selma 2005).

The main activity in the area is agriculture with 858,000 ha of crops from which 230,000 are irrigated (Montesinos et al. 2009), and is the principal source of water demand. Presently, the amount of water used for irrigation is estimated to approximately 1,400 hm³, representing more than 70% of the total water demand of the SRB.

▪ *Sites description (Calasparra, Jumilla, Murcia)*

Calasparra

Of the three SRB weather station sites, Calasparra is the only one that is entirely surrounded by rural area (Figure 12). The pixel comprises, mainly fruit trees and berry plantations (Figure 13). The annual rainfall is around 330mm and the average temperature is 16°C. The type of soil in the area is a mixture of gleic solonchacks, petrocalcium xerosols, calcium regosols, calcium fluvisols and litosols.

Figure 12: Areal view of Calasparra site from Google maps. The green arrow represents the weather station and the red square represents MODIS pixel that was considered in this study for this site.

Figure 13: Land use map from the CORINE Land cover map (2006) of the surrounding area of the Calasparra site.

Jumilla

The Jumilla weather station is located on the edge of an urban fabric area (Figure 14). The pixel comprises, in its Northern part, the urban nucleus of Jumilla, and in its southern part, agricultural fields with mixed crops, mostly non-irrigated (Figure 15). The annual rainfall in Jumilla is around 305mm and the average temperature is 15°C. The type of soil in the area is a mixture of gleic solonchacks, petrocalcium xerosols and calcium xerosols.

Figure 14: Areal view of Jumilla site from Google maps. The green arrow represents the weather station and the red square represents MODIS pixel that was considered in this study for this site.

Figure 15: Land use map from the CORINE Land cover map (2006) of the surrounding area of the Jumilla site.

Murcia

The Murcia weather station (Figure 16) is also located on the border between an urban and an agriculture area, mostly irrigated as opposed to Jumilla's site. The annual rainfall in Murcia is around 300mm and the average temperature is 18°C. The type of soil in the area is mainly calcium fluvisols.

Figure 16: Areal view of Murcia site from Google maps. The green arrow represents the weather station and the red square represents MODIS pixel that was considered in this study for this site.

Figure 17: Land use map from the CORINE Land cover map (2006) of the surrounding area of the Murcia site.

▪ ***Meteorological data***

The meteorological data were provided by the SIAM weather station network. The SIAM (Sistema de Información Agrario de Murcia) is the Murcia Region's System of Information for Agriculture. All weather stations are equipped with the equipment described in Table 2, providing mean-hourly data. The data used in this study was mainly relative humidity, precipitation, air temperature and solar radiation.

Table 2: *Meteorological instrumentation at the sites*

Brand	Model	Description
YOUNG	05103-5	WIND MONITOR
KIPP & ZONEN	CMP6	RADIOMETER
GEONICA (Murcia) THIES-CLIMA (Calasparra and Jumilla)	PCP-214 5.4031.30.007	PLUVIOMETER
CAMPBELL	CR1000	DATALOGGER
VAISALA	HMP45AC	THERMO-HYGROMETER

3.2.3. Mar Menor lagoon

▪ *Site description*

Mar Menor is a sheltered hypersaline lagoon located in Murcia Region, in the River Segura Basin (Figure 18). It is one of the largest coastal lagoons in the Mediterranean region as well as in Europe. The lagoon has a maximum depth of 7.0 m and a mean depth of 4.5 m. The surface area is 135.5 km², the perimeter is 74 km and the total volume of water in the lagoon is 610 hm³. 'La Manga', a sandbar 23 km in length with a maximum width of 900 m, acts as a barrier between the lagoon and the Mediterranean Sea. Five shallow channels in the sandbar connect the lagoon with the open sea. The coastline is low-lying, with sandy or rocky beaches.

Figure 18: Map and bathymetry of the Mar Menor coastal lagoon, including location of the meteorological station E1 (San Javier) and the marine buoys B1 (Mar Menor) and B2 (Mediterranean Sea).

The climate is of typical semi-arid Mediterranean like in the rest of River Segura Basin's coastal area, with mean annual temperatures ranging from 15 to 17 °C. The mean annual rainfall is approximately 300 mm with most precipitation occurring in short-episodic storm events in the autumn and the winter. The mean reference evapotranspiration, estimated by means of the Penman-Monteith method (Allen et al.

1998), is approximately 1350 mm y⁻¹. Thus, the net hydrologic balance of the lagoon reaches annual deficits close to 1000 mm y⁻¹, which are compensated for by freshwater inflows and by saltwater from the sea.

The Spanish Mediterranean coast has semidiurnal tides with small amplitude. The lunar tide in the study area, predicted by the CEFMO model (Legos) is approximately 0.1 m. However, daily pressure fluctuations and wind stress drive barotropic tides resulting in total daily tide amplitudes ranging from 0.2 to 0.4 m. There are also seasonal pressure fluctuations that produce small seasonal variations in the mean level of the Mediterranean Sea but there is not a clear seasonal variability pattern.

Water exchanges are regulated by differences in the sea level between the lagoon, which has no appreciable water level variations, and the open sea, which is subjected to tidal dynamics. The average lagoon water renewal time is approximately 1.2 years (FIEA 2009) and its circulation is mainly conducted by wind (Pérez-Ruzafa et al. 2005).

The Mar Menor watershed constitutes a wide (1,200 km²) sedimentary plain with sediments of Neogene and Quaternary that are slightly inclined to the Mar Menor. The main materials constituting this basin are conglomerates, marls, sandstones, slimes and clays, resulting in high soil diversity due to the heterogeneity of geologic conditions (Martínez et al. 2004). The lagoon is influenced by the watershed through surface and groundwater flows.

The relative isolation of Mar Menor from the Mediterranean Sea implies that the seasonal fluctuations of the environmental factors are much more marked in the lagoon than on the marine coast. This is evident in Rosique (2000)'s review of Mar Menor data availability, which shows that while the lagoon water temperature presents a regular seasonal cycle between 10 and 11 °C in January and 29 and 30 °C in August, the Mediterranean Sea temperature only varies between 13 and 27 °C. Furthermore, these minimum and maximum values are delayed by a month from those of Mar Menor.

▪ ***Meteorological and hydrological data***

The meteorological data required to run the model (described in Chapter 6, Section 6.4.1.) were daily air temperature (T_a) and relative humidity (RH), precipitation (P), wind speed (U) and solar global radiation (R_s) for the period from 2003 to 2006. Data were obtained at the meteorological station of the San Javier airport (37°47'12"N 0°48'08"W, height: 2 m above sea level), located at the lagoon's north-west coast (Figure 18). All data were measured at a height of 2 m aboveground with the exception of wind, which was measured at 10 m and corrected to derive the values at 2 m following the equation proposed by Allen et al. (1998).

The water balance inflows are precipitation, runoff and groundwater discharges, as well as incoming water from the sea. The outflows are evaporation and the outgoing water to the sea. Daily water exchanges with the sea and evaporation in the lagoon were estimated by solving the daily water balance equation and are discussed in Chapter 6. Runoff and groundwater discharges were evaluated as follows.

The watershed is drained by more than twenty riverbeds that are constituted by ephemeral channels. The main collector in the drainage basin (*El Albuñón* watercourse) maintains a regular flux fed by exfiltrated groundwater, which is only continuous in the last 5–8 km, depending on the season. The baseflow in the mouth of the basin is generally around $0.02 \text{ m}^3 \text{ s}^{-1}$ ($0.63 \text{ hm}^3 \text{ y}^{-1}$). However, during a typical storm event (return period of 5 years) the flow rapidly increased up to $10.5 \text{ m}^3 \text{ s}^{-1}$ and returned close to its baseflow level within less than 24 h (García-Pintado et al. 2007). The total runoff discharge in the lagoon was recently estimated between 5 and $8 \text{ hm}^3 \text{ y}^{-1}$ (MIMAM 2007), but there are no daily records to support these data. Considering the lack of reliable records of daily runoff discharge, as well as the irregularity and relative low impact on the water budget, this inflow was disregarded in the study.

In relation to sub-surface hydrology, Mar Menor also receives subterranean flow contributions from the west, but only those belonging to the upper Quaternary aquifer, because the deeper aquifers (Triassic, upper Miocene, and Pliocene) are hydrogeologically disconnected due to the action of coastal faults (Rodríguez-Estrella 2004). There is a coastal groundwater discharge along the contact front (30 km length, $\approx 5 \text{ m}$ depth) between the Quaternary aquifer and the lagoon as well as direct agricultural drainage channel discharges (Rodríguez-Estrella 1995). The magnitude of these flows was recently estimated to be 7.6 and $18.3 \text{ hm}^3 \text{ y}^{-1}$, respectively (FIEA 2009).

The piezometric network in the Mar Menor watershed (CHS 1998) consists of 14 controlled wells with data from 1975 to the present. Their piezometric height remained stable during the last decade, resulting in a soft and constant hydraulic gradient ($4.5 \cdot 10^{-3} \text{ m m}^{-1}$) that indicates that the groundwater discharge can be considered uniformly distributed throughout the year. Therefore, the groundwater discharge considered in this study was a daily constant value of $(7.6 + 18.3)/365 = 71 \cdot 10^{-3} \text{ hm}^3 \text{ d}^{-1}$. It is assumed that this amount includes the watercourse's baseflow ($0.63 \text{ hm}^3 \text{ y}^{-1}$) because it comes from exfiltrated groundwater.

Data of water exchange with the Mediterranean Sea are available only for the major connection channel (*El Estacio*). Arévalo (1988) indicated that the exchange through *El Estacio* presented a high fluctuant regime of currents with a frequent inversion of the direction of flows, which was regulated by the Mediterranean tidal dynamics. He further reported that the total water exchange reached a value of approximately $1.6 \text{ hm}^3 \text{ d}^{-1}$ and was considerably higher than throughout the remainder of the channels.

3.3. Satellite data

3.3.1. The MODIS-Terra and Aqua EO satellite

All the remote sensing data used in this work were obtained from images and products of the Moderate-resolution Imaging Spectroradiometer sensor (MODIS).

MODIS was launched into Earth orbit by NASA in 1999 on board the Terra (EOS AM) Satellite as one of the five sensors onboard, and in 2002 on board the Aqua (EOS PM) satellite. Terra's orbit around the Earth is timed so that it passes from north to south across the equator in the morning, while Aqua passes south to north over the equator in the afternoon. The instruments capture data in 36 spectral bands ranging in wavelength from 0.4 μm to 14.4 μm and at varying spatial resolutions (2 bands at 250 m, 5 bands at 500 m and 29 bands at 1 km). Together the instruments image the entire Earth every 1 to 2 days.

Figure 19: Illustration of spatial platform Terra and Aqua that shelter MODIS sensor.

3.3.2. MODIS products used in the studies

The images used in this study are from MODIS-Terra sensor for Land Surface Temperature (LST) and Normalized Difference Vegetation Index (NDVI) products, and from MODIS-Aqua sensor for the Sea Surface Temperature (SST). MODIS products are available freely for the science community which makes its use very attractive. The

products used are MOD11A1 (LST product), MOD13A2 (Vegetation Indices), and MOD 28 (SST product), all of them at a 1 km spatial resolution.

The MOD11A1 product is produced daily using the generalized split-window LST algorithm. The split window method is used to retrieve the LST based on the differential water vapor absorption in two adjacent infrared channels.

The MOD11A1 product comprises the following Science Data Set (SDS) layers for daytime and nighttime observations: LSTs, quality control assessments, observation times, view zenith angles, clear sky coverages, and bands 31 (10.780–11.280 μm) and 32 (11.770–12.270 μm) emissivities from land cover types.

Global MODIS vegetation indices (MOD13A2 product) are designed to provide consistent spatial and temporal comparisons of vegetation conditions. Red, and near-infrared reflectances, centered at 645-nanometers, and 858-nanometers, respectively, are used to determine the MODIS daily NDVI.

MODIS NDVI product is computed from atmospherically corrected bi-directional surface reflectances that have been masked for water, clouds, heavy aerosols, and cloud shadows. NDVI is calculated with the following equation:

$$NDVI = \frac{NIR - Red}{NIR + Red} \quad (18)$$

where *NIR* is the reflectance the near-infrared band and *Red* is the reflectance in the red band.

Global MOD13A2 data are available every 16 days at 1-kilometer spatial resolution.

MODIS SST product (MOD38) is available on a daily basis at 1-kilometer spatial resolution. Sea surface temperature determination is based on MODIS-calibrated mid- and far-IR radiances (Bands 20, 22, 23, 31, and 32 from MOD 02), using an algorithm that exploits the differences in atmospheric transmissivity in the different IR bands to enable highly accurate estimation of the atmospheric effects, thereby enabling ancillary input to the algorithm along with a land mask, which is used to mark nonwater pixels.

3.2.3. Satellite image Processing

Processing of the MODIS-Terra (LST and NDVI) images after acquiring them consisted in cutting out the zone of interest using the Modis Reprojection Tool, followed by a filtering to extract only the pixels with acceptable quality using the quality flags provided with each image. For LST images, the pixels for which the zenith angle of pixel view was greater than 30° were rejected as they are considered not enough reliable according to Wang et al. (2008). According to these authors, LST data with zenith viewing angle <30 have average errors 0.5-0.8 degrees lower than with zenith viewing angle >30 .

For MODIS-Aqua MOD38 Sea Surface Temperature product, the software SeaDas 5.1 was used to process the images. The quality level ranges from 0 for the best quality to 4 for the worst quality. For this study, only pixels with quality levels between 0 and 2 were selected.

The MODIS-Aqua daily daytime images were taken in the study area between 12:30 and 14:00 GMT. The observed surface varied depending on the date and hence affected the availability of representative pixels of Mar Menor and its vicinity. Eighteen different types of images, corresponding to different satellite overpass times, were found for the study period (2003 to 2006). For each type of image, a macro was programmed to automatically filter the data and to calculate the mean temperature of the Mar Menor surface (T_w) and the selected vicinity of the Mediterranean Sea ($T_{w, Med}$).

3.4. Selected ET retrieval method: the triangle method

The selected retrieval method is the so-called “triangle” method (see Section 2.2.), in its version described by Jiang and Islam (2001). This method avoids complicated parameterizations that involve heat and momentum resistances to energy transfer for ET estimation, and numerous correction procedures (Jiang et al. 2009). The retrieval of ET is based on the estimation of evaporative fraction (EF) using the distribution of the T_s –NDVI spatial variation, where T_s is the land surface radiometric temperature (LST from MODIS in our case) and NDVI is the Normalized Difference Vegetation Index provided by satellite data. It is called the “triangle” method, for the spatial variation of the T_s and NDVI often results on a triangle shape (Figure 20). For wet, vegetated surfaces, evapotranspiration is at its maximum, cooling down the surface temperature. Therefore, the lower limit of the triangle is called the “cold edge” or “wet edge”, and corresponds to the pixels with the highest values of EF. On the other hand, the dry surfaces constitute the upper limit of the triangle called “warm edge” or “dry edge” with higher temperature that increase in bare soil, and where EF is at its minimum.

Figure 20: T_s -NDVI space in the triangle method.

In Jiang and Islam (2001), the basic assumption is that the interior of the VI - T_s space scales linearly with the surface energy fluxes.

The method is based on an extension of the Priestley Taylor equation (Priestley and Taylor 1972) and a relationship between remotely sensed surface temperature and vegetation index to estimate ET.

$$ET = \phi \left(\frac{\Delta}{\Delta + \gamma} \right) (R_n - G) \quad (19)$$

where ET is the latent heat flux ($W\ m^{-2}$), R_n is the net radiation ($W\ m^{-2}$), G is the soil heat flux ($W\ m^{-2}$), ϕ is the parameter that accounts for aerodynamic and canopy resistance, Δ is the slope of saturated vapour pressure at air temperature (T_a) and γ is the psychrometric constant.

The basis of the methodology is the existence of a physically meaningful relationship between ϕ values and a combination of remotely sensed spatial parameters, T_s (surface temperature) and NDVI (the Normalized Difference Vegetation Index).

Figure 21 shows a conceptual diagram of Jiang and Islam (2001) version. $\phi_{min}=0$ corresponds to the driest bare soil pixel and $\phi_{max}=1.26$ for the densely vegetated pixel. Given these two bounds, $\phi_{i,min}$ for each $NDVI_i$ can be linearly interpolated, and $\phi_{i,max}$ can be obtained from the pixel corresponding to the lowest surface temperature within each NDVI interval. ϕ for every individual pixel can be calculated interpolating between the lowest and the highest surface temperature within that NDVI class.

Figure 21: Conceptual diagram of the triangle method in Jiang and Islam (2001) version.

The “triangle” method was first introduced by Price (1990) and later elaborated upon by Carlson et al. (1994, 1995) Gillies and Carlson (1995), Lambin and Ehrlich (1996), Gillies et al. (1997), Owen et al. (1998), Jiang and Islam (1999, 2001, 2003) and Jiang et al. (2004). This method was adopted and successfully applied to retrieve EF, ET and soil moisture by a number of researchers. Toby Carlson (2007) gives an overview of the use of the “triangle” method for estimating ET and soil moisture, and shows how the triangle can be recreated from a land surface model. The use of an “universal triangle” is also explored, to see how a single pixel’s position within the triangle can be interpreted, and how land use change is traduced into specific trajectories of that single pixel within the triangle.

3.5. The JULES land surface model

The land surface model (LSM) used for this study is the Joint UK Land Environment Simulator (JULES), developed from the Met Office Surface Exchange Scheme (MOSES). It can be used as a stand alone land surface model driven by observed forcing data, or coupled to an atmospheric global circulation model.

JULES has a tiled model of sub-grid heterogeneity with separate surface temperatures, shortwave and long-wave radiative fluxes, sensible and latent heat fluxes, ground heat fluxes, canopy moisture contents, snow masses and snow melt rates are computed for each surface type in a grid-box. Nine surface types are recognized: broadleaf trees, needleleaf trees, C3 (temperate) grass, C4 (tropical) grass, shrubs, urban, inland water, bare soil and ice. Except for those classified as land-ice, a land grid-box can be made up from any mixture of the first 8 surface types. Fractions of surface types within each land-surface grid-box are read from an ancillary file or modelled by the dynamic global vegetation model TRIFFID (Top-down Representation of Interactive Foliage and Flora Including Dynamics). In our case, the TRIFFID model was turned off, as the time period considered was not long enough to involve vegetation dynamic processes.

Air temperature, humidity and windspeed on atmospheric model levels above the surface and soil temperatures and moisture contents below the surface are treated as homogeneous across a grid-box.

A schematic diagram of the modular structure of JULES is represented in Figure 22.

Although all the modules are interconnected and linked in JULES, in this study, we are mainly focusing on surface fluxes. Therefore, in this section, the emphasis is placed on the description of the surface exchange module (which estimates the energy fluxes). This is followed by a brief summary of the photosynthesis treated in the plant physiology module, because the latter provides the value of surface conductance to the surface exchange module (see Figure 22). At last, plant transpiration is presented. For the rest of modules, the reader is referred to the two companion papers Best et al. (2011) and Clark et al. (2011).

Figure 22: From Best et al. (2011). Modular structure of JULES model. The Boxes show each of the physic modules whilst the lines between the boxes show the physical processes that connect these modules. The surrounding three boxes show the cross-cutting themes.

3.5.1. Energy balance

In the standard surface energy balance equations, used to calculate the distribution of available energy between the various fluxes at the surface, thermal inertia is associated with the surface mass which is coupled to the underlying soil by three physical mechanisms depending upon the type of surface. The vegetation fraction is coupled to the soil using radiative exchange and atmospheric turbulence, whereas the remainder are coupled through conduction.

The surface energy balance equation is then written:

$$C_s \frac{\delta T_*}{\delta t} = (1 - \alpha) S W_{\downarrow} + \epsilon L w_{\downarrow} - \sigma \epsilon (T_*)^4 - H - L_c - G \quad (21)$$

where:

$$H = \frac{\rho c_p}{r_a} (T_* - T_A) \quad (22)$$

$$E = \frac{\rho}{r_a + r_s} (Q_{sat}(T_*) - Q_l) \quad (23)$$

$$G = v \left[\sigma \epsilon \epsilon_s (T_*)^4 - \sigma \epsilon \epsilon_s (T_{sl})^4 + \frac{\rho c_p}{r_{a_{can}}} (T_* - T_{sl}) \right] + (1 - v) \lambda_{soil} (T_* - T_{sl}) \quad (24)$$

where the definition for the symbols are (in alphabetical order):

c_p is the specific heat capacity of air ($\text{J kg}^{-1} \text{K}^{-1}$);

C_s is the areal heat capacity associated with the surface material ($\text{J m}^{-2} \text{K}^{-1}$);

E is the turbulent moisture flux ($\text{kg m}^{-2} \text{s}^{-1}$);

G is the soil heat flux (W m^{-2});

H is the turbulent heat flux (W m^{-2});

L_c is latent heat of condensation of water at 0°C ;

$Lw_{\downarrow}$ is the downward component of the longwave radiation (W m^{-2});

Q_l is the specific humidity at the reference atmospheric level (kg kg^{-1});

$Q_{\text{sat}}(T_*)$ is the saturated specific humidity at the temperature T_* (kg kg^{-1});

T_* is the surface temperature (K);

T_A is the reference level atmospheric temperature (K);

T_{sl} is the temperature of the first soil level (K);

r_a is the aerodynamic resistance (s m^{-1});

$r_{a_{can}}$ is the aerodynamic resistance between the surface canopy (s m^{-1});

r_s is the stomatal or surface moisture resistance (s m^{-1});

$Sw_{\downarrow}$ is the downward component of the solar radiation (W m^{-2});

α is the surface albedo;

ϵ is the surface emissivity;

ϵ_s is emissivity of the underlying soil surface;

λ_{soil} is the thermal conductivity of the soil ($\text{W m}^{-1} \text{K}^{-1}$);

v is the fraction of vegetation;

ρ is the density of air (kg m^{-3});

σ is Stefan Boltzmann constant ($\text{W m}^{-2} \text{K}^{-4}$).

The surface heat capacity is specified for non-vegetation surfaces, but is determined from the leaf and woody biomass for vegetation using:

$$C_s = C_L B_L + C_W B_W \quad (25)$$

where C_L is the specific heat capacity of leaves ($\text{J kg}^{-1} \text{K}^{-1}$); B_L is the leaf biomass (kgC m^{-2}); C_W is the specific heat capacity of wood ($\text{J kg}^{-1} \text{K}^{-1}$); and B_W is the wood biomass (kgC m^{-2}).

Larger heat capacities result in a stronger thermal inertia for the surface.

The aerodynamic resistance is calculated using standard Monin-Obukhov similarity theory (Monin and Obukhov 1954), using the stability functions of Dyer (1974) for unstable conditions and Beljaars and Holtslag (1991) for stable conditions. The surface resistance for surfaces with potential evaporation (i.e., lake, snow and ice surfaces) is set to zero, whilst for an urban surface the conductance is set to zero unless water is available on the urban surface (i.e., the urban “canopy water”). For a bare soil surface, the surface conductance (g_{soil} , inverse of resistance) is determined by the soil moisture concentration in the top soil layer:

$$g_{soil} = \frac{1}{100} \left(\frac{\theta_l}{\theta_c} \right)^2 \quad (26)$$

where θ_l is the soil moisture concentration on the top soil layer ($\text{m}^3 \text{m}^{-3}$) and θ_c the soil moisture concentration at critical point ($\text{m}^3 \text{m}^{-3}$). The critical point is that at which soil moisture stress starts to restrict transpiration.

For vegetation, the surface resistance is calculated using the photosynthesis model described in next section.

For the vegetative surfaces, the latent heat flux is determined from a combination of evapotranspiration and bare soil evaporation. The relative contributions from vegetation and bare soil are a representation of the fraction of bare soil that can be seen through the vegetation canopy. Hence the fractions for each of these are determined by the density of the leaves, through the leaf area index. The combined flux represents the interaction of the atmosphere with both the canopy and the soil beneath.

3.5.2. Photosynthesis module

The leaf level stomatal conductance (g_s) and net photosynthetic uptake (A) are linked via the CO_2 diffusion equation:

$$A = g_s(C_c - C_i)/1.6 \quad (27)$$

where C_c is leaf surface carbon dioxide concentration (Pa) and C_i is internal leaf carbon dioxide concentration (Pa).

Leuning (1995) stomatal conductance formulation relates the ratio of internal to external CO_2 concentrations to leaf humidity deficit:

$$\frac{C_i - C_*}{C_c - C_*} = f_0 \left(1 - \frac{D}{D_*} \right) \quad (28)$$

where C_* is CO_2 compensation point (Pa) (the compensation point is the concentration of atmospheric carbon dioxide at which the rate of carbon dioxide uptake by a photosynthesizing plant is exactly balanced by its rate of carbon dioxide release in respiration and photorespiration); D is the leaf humidity deficit (kg kg^{-1}). D_* and f_0 are vegetation specific calibration parameters, which are directly related to the parameters from the Leuning (1995) model (for details, see Cox et al., 1998).

This simplified formulation is convenient for large scale model applications (Cox et al. 1998). Potential (non-water stressed) leaf level photosynthesis (A_P) is calculated in JULES using the C3 and C4 photosynthesis models of Collatz et al. (1991) and Collatz et al. (1992) respectively. Photosynthesis is simulated as the minimum of three limiting rates: (i) Rubisco limited rate (W_C), (ii) light limited rate (W_L) and (iii) rate of transport of photosynthetic products (in the case of C3 plants) and PEP-Carboxylase limitation (in the case of C4 plants) W_E , with both, W_C and W_L having a dependency on the leaf internal CO_2 concentration, C_i .

$$A_P = \min(W_C, W_L, W_E) \quad (29)$$

Leaf photosynthesis A , is related to the potential (nonstressed) leaf photosynthesis (A_P) as follows,

$$A = A_P \beta \quad (30)$$

β is the dimensionless moisture stress factor, which is related to the mean soil moisture concentration in the root zone, and the critical and wilting point concentrations as follows:

$$\beta = \begin{cases} 1 & \text{for } \theta \geq \theta_c \\ \frac{\theta - \theta_w}{\theta_c - \theta_w} & \text{for } \theta_c \leq \theta \leq \theta_w \\ 0 & \text{for } \theta \leq \theta_w \end{cases} \quad (31)$$

where θ is soil moisture concentration ($\text{m}^3 \text{m}^{-3}$); θ_c is soil moisture concentration at critical point ($\text{m}^3 \text{m}^{-3}$); and θ_w is soil moisture concentration at wilting point ($\text{m}^3 \text{m}^{-3}$).

The critical point is defined by a matrix water potential of -33 kPa (Cox et al. 1999), and enables vegetation to maintain an un-water stressed transpiration at values below field capacity.

In this study, the option selected for up-scaling to canopy level was the multilayer approach, which is more realistic than the “big-leaf” approach (Mercado et al. 2007). In the multilayer approach, the radiation absorbed and photosynthesis are estimated using a user defined number of leaf area increments (canopy layers) within the canopy, with the total canopy level flux calculated as the sum of the fluxes from each individual canopy layer (Jogireddy et al. 2006; Mercado et al. 2007).

3.5.3. Transpiration module

The ability of vegetation to access moisture at each level in the soil is determined by root density, assumed to follow an exponential distribution with depth. The fraction of roots in soil layer k extending from depth z_{k-1} to z_k is

$$r_k = \frac{e^{-2z_{k-1}/d_r} - e^{-2z_k/d_r}}{1 - e^{-2z_t/d_r}} \quad (32)$$

where r_k fraction of roots in the k -th soil layer; z_t is the total depth of soil column (m); z_k and z_{k-1} are depth of the k -th and $(k-1)$ -th soil layers respectively (m); and d_r is the root depth (m).

For transpiration E' , the flux extracted from soil layer k is $e_k^0 E'$, where

$$e_k^0 = \frac{r_k \beta_k}{\sum_k r_k \beta_k} \quad (33)$$

and

$$\beta_k = \begin{cases} 1 & \text{for } \theta_k \geq \theta_c \\ \frac{\theta_k - \theta_w}{\theta_c - \theta_w} & \text{for } \theta_c \leq \theta_k \leq \theta_w \\ 0 & \text{for } \theta_k \leq \theta_w \end{cases} \quad (34)$$

is a soil moisture availability factor, defined similarly to Eq. (31), for a soil layer with unfrozen volumetric soil moisture concentration k .

3.5.4. Accounting for surface heterogeneity

The heterogeneity of the surface is modelled within JULES by using the tile, or mosaic, approach (e.g., Essery et al. 2003). This means that a separate surface energy balance is determined for each type of surface within the domain of the gridbox or footprint, and the individual surface fluxes are then given a weighted average in order to determine the gridbox or footprint mean flux into the atmosphere. One limitation to the current structure of JULES is that although the surface exchange represents the

heterogeneity through tiling, there is no representation of sub-gridscale heterogeneity within the sub-surface soil module.

There are two generic types of surface in JULES having differing requirements for their surface parameters: (1) Nonvegetated surfaces with fixed parameter values (e.g., albedo and roughness length) which are specified at run time, and (2) vegetated surfaces whose parameters vary. The roughness length for momentum for vegetation is determined from

$$z_0 = \omega h \quad (35)$$

where ω is the rate of change of roughness length with vegetation canopy height (m m^{-1}).

For the calculation of surface albedo (α), the snow-free albedos are calculated using the two-stream model for radiative transfer through vegetation described by Sellers et al. (1992). This scheme uses separate direct-beam and diffuse albedos in the visible and near-infrared wave bands for each vegetation type. This requires four parameter values for leaf reflection coefficients and leaf scattering coefficients for both near infra-red and photosynthetically active radiation.

An additional parameter for vegetation surfaces is the capacity of the canopy to hold water (C_m) through the interception of precipitation,

$$C_m = A_m + B_m L \quad (36)$$

where A_m is the puddling of water on soil surface and interception by leafless vegetation (kg m^{-2}); B_m is the rate of change of water holding capacity with leaf area index (kgC m^{-2}); and L is the leaf area index ($\text{m}^{-2} \text{m}^{-2}$).

By default nine surface types are represented; five vegetation (broadleaf trees, needleleaf trees, C3 grasses, C4 grasses and shrubs) and four non-vegetated surfaces (urban, open water, bare soil and permanent land ice).

3.5.5. Forcing data and ancillary files

In this study, JULES was forced by the Princeton data set, described in Sheffield et al. (2006). The Princeton data set is a global, 50-yr, 3-hourly, 1.0° dataset of meteorological forcings that can be used to drive LSMs. The driving data needed by JULES are precipitation (rainfall and snowfall), shortwave and longwave downscale radiation, near-surface air temperature, near surface specific humidity, wind speed, and air pressure.

The ancillary information necessary is:

- Land cover: nine surface types are represented; five vegetation (broadleaf trees, needleleaf trees, C3 grasses, C4 grasses and shrubs) and four non-vegetated surfaces (urban, open water, bare soil and permanent land ice), and each grid-box (ice-free) can be a combination of the eight first surface types. The land cover map used in this work is the one generated by the MetOffice central ancillary file maker, and is based on IGBP (International Geosphere-Biosphere Programme) land cover product, described in Belward et al. (1999).

- Soil properties:

Thermal properties of the soil are the one described in Dharssi et al. (2009).

Hydraulic properties: One of the options of JULES that was chosen regarding soil properties was to switch the Van Genuchten soil hydraulic model on to estimate the conductivity of unsaturated soils (Van Genuchten 1980). The Van Genuchten parameters for the different type of soils are derived from the HYPRES (HYdraulic PROPERTIES of European Soils) data base, described in Wösten et al. (1999).

Chapter 4: A new parameterisation scheme of conduction heat flux

4.1. Introduction

Chapter 1 emphasized the importance of estimating surface fluxes, especially ET, for many applications in hydrology, agriculture, meteorology, climate modelling, and water management, among others. In Chapter 2, we presented current techniques to estimate those fluxes, and made clear the strategic importance of RS-data and flux-retrieval methods for spatialising ET estimates. Although significant progress has been achieved in ET mapping from EO information in the past decades, it should be recognised that the estimation of ground heat flux, G , is still a pending issue. This flux can reach high values in arid and semiarid areas, and a robust estimate of G is necessary to determine realistically the energy partitioning at the ground.

Ground truth validation of flux-retrieval algorithms is not straightforward because of the difficulty in obtaining reliable pixel-averaged values (e.g. 1 km²) of the SEB components. If relatively accurate ground measurements of area-averaged ET and H can be obtained, generally by means of the eddy-covariance flux-towers (Scott 2010; Mu et al. 2007; McCabe and Wood 2006), the issue of getting reasonably-accurate measurements of area-averaged soil heat flux, G , is still to be resolved. The two main causes of the large errors in measuring are (i) the recognised lack of accuracy of the G measurement methods (see, among others, Ochsner et al. 2006) and (ii) the large number of sampling points in sparse vegetation covered areas. Even with a large network of sensors around the flux-tower, the footprint of G measurements remains very small compared to the footprint of the fluxes measured by eddy correlation (Schüttemeyer et al. 2006). The combination of the two types of errors results generally in rather imprecise ground data of G , and to large uncertainties when upscaling from point measurements to EC footprints or to large pixels.

Prediction of G can be improved by means of analytical or numerical tools based on the resolution of the heat diffusion equation. These methods are physically-based and therefore are universal, but highly demanding in input data and rather complex to handle.

The alternative to numerical methods is the empirical approach based on experimentally-derived relationships between G and one of the components of the surface energy balance equation. In Chapter 2, section 2.2.1., common approaches to estimate G in past and current works based on RS are presented, which are mainly G expressed as a function of net radiation R_n alone or combined with vegetation (through NDVI for example) or alternatively, G as a function of sensible heat flux. Although all these methods are commonly used, they have been criticised for lacking precision (Clothier et al. 1986; Santanello and Friedl 2003; Fuchs and Hadas 1972; Idso et al. 1975; Ogée et al. 2001; Cellier et al. 1996).

In this study, we hypothesised that more realistic estimates of G could be obtained by directly linking the parameter $\alpha = G/R_n$ to the evaporative fraction, EF , the latter being more responsive than VIs to soil moisture in sparse vegetated areas. We first demonstrated that the parameters α and $\gamma = G/H_s$ are linked to the evaporative fraction by a functional relationship, and that both could be expressed as a function of EF , therefore providing a theoretical basis for our basic assumption. In a second step, we proposed an EF -based parameterisation of α , using ground flux data sets obtained at four flux-tower sites in West African countries (Mali, Benin, Niger) that differ in surface conditions and Monsoon influence. Those sites were described in Chapter 3. Finally, we investigated whether the ET-retrieval method using the new parameterisation of α could perform better than the classical formulation through VI-based relationships.

4.2. Basis of the parameterisation scheme

The evaporative fraction EF is defined as:

$$EF = ET / (R_n - G) \quad (37)$$

Expressing the ground heat flux as a function of net radiation

$$G = \alpha R_n \quad (38)$$

and sensible heat flux

$$G = \gamma H \quad (39)$$

and rearranging with Eqs. 1 (energy balance equation presented in Chapter 1) and 37 supplies the following functional relationships between EF, α and γ :

$$EF = 1 - \frac{1}{\gamma} \frac{\alpha}{1 - \alpha} \quad (40)$$

$$\alpha = \frac{\gamma(1 - EF)}{1 + \gamma(1 - EF)} \quad (41)$$

$$\gamma = \frac{\alpha}{(1 - \alpha)} \frac{1}{(1 - EF)} \quad (42)$$

It should be noted that Eqs. 40, 41 and 42 are alternative – and equivalent – formulae to express the surface energy balance (Eq. 1) in a non-dimensional form through EF, α and γ . Eq. 40 indicates that EF decreases with increasing α for a fixed γ value and increases with increasing γ for a fixed α value (Figure 23). Note that:

- for a given value of EF, there are several pairs of values (α, γ) that could be solution of the equation
- for high positive values of γ , EF tends towards 1 and is practically insensitive to α
- EF and α being positive during daytime, their values could be constrained within realistic lower and upper limits, whereas γ is not constrained – like the Bowen ratio – and could reach very high values ($H \approx 0$) or could be negative ($H < 0$) in case of local advection process (Figure 23).

In this study, ground data were available of the ratio H/R_n , which is equal to α/γ :

$$\frac{H}{R_n} = \frac{H}{G} \times \frac{G}{R_n} = \frac{\alpha}{\gamma} \quad (43)$$

We have therefore two equations (Eqs. 41 and 42) for three unknowns. It is necessary to make a plausible assumption about one of the unknowns to compute the two others. For the dry season, it was assumed that EF was equal to 0 (section 4.3.1.). For the wet season, a plausible predetermined value of γ was used (section 0.). Once the parameters were identified at each site (hereafter, with subscripts 'wet' and 'dry' respectively for the wet and dry season), they can be plotted in the EF- α (or EF- γ) space and used to derive a possible general relationship between the site-average values of EF and α - or γ - that can be used to predict G from EF. These mean seasonal values of EF, α and γ characterise the average energy balance at each site.

Figure 23: Graphical representation of Eq. 40 showing the dependency of EF on α for different γ values. The two arrows represent plausible ranges for α at high EF ($EF > 0.75$) and low EF ($EF \approx 0$). Negative values of γ correspond to advective conditions ($EF > 1$). The thick curve represents the relationship between EF and α for $\gamma = 0.3$. The parameter α was constrained to the interval $0 < \alpha < 0.6$.

4.3.Parameter identification

4.3.1. Dry season

EF at the apogee of the dry season can be assumed to be equal to zero at the Sahelian sites (Banizoumbou, Eguerit and Kelma). For $EF = 0$, we get:

$$\gamma_{dry} = \frac{\alpha_{dry}}{1 - \alpha_{dry}} \quad (44)$$

That is, as $H_{dry}/R_{n,dry} = \alpha_{dry}/\gamma_{dry}$, $R_{n,dry}$ being the value of the net radiation observed at the time H_{dry} occurred, we get

$$\alpha_{dry} = 1 - \frac{H_{dry}}{R_{n,dry}} \quad (45)$$

We calculated α_{dry} and γ_{dry} from the ground data sets for the 15 highest values of the ratio $H_{dry}/R_{n,dry}$ observed at 11h (MODIS-Terra overpass time) at the four sites and for sunny days of the dry season. The average value and standard deviation of the 15 values of α_{dry} and γ_{dry} at 11h were determined. For the semi-tropical site (Bellefoungou), evaporation during the dry season was small, yet not negligible and EF cannot be taken as 0. We therefore determined a proxy for EF_{dry} using the minimum value of EF provided by the triangle method ($EF_{dry} \sim 0.15$), and derived the corresponding values of α_{dry} and γ_{dry} at Bellefoungou, corresponding to the 15 highest values of $H_{dry}/R_{n,dry}$. The normalised difference vegetation index ($NDVI_{dry}$) and ground albedo (a_{dry}) and their standard deviations were calculated for the same days.

4.3.2. Wet (monsoon) season

To identify the parameter values in the wet season, for which EF values were unknown, it was necessary to guess a plausible mean value of one of the two other unknowns, α or γ . Under high evapotranspiration rate, α is generally small, varying in the interval $0 < \alpha < 0.10$. In this range, the assumption that γ is close to 0.30 might be quite realistic (Figure 23). We therefore derived the instantaneous and mean values of EF and α using this assumption. In a similar way to the procedure applied for the dry season, we selected the 15 days with the lowest value of the ratio $H_{\text{wet}}/R_{n,\text{wet}}$, which were likely to correspond to the days with the highest evaporation fraction at each site.

4.3.3. Retrieved values of H

Replacing G by αR_n in the energy balance equation and rearranging, H_r was obtained from:

$$H_r = (1 - \alpha)(1 - EF_T)R_n \quad (46)$$

where EF_T is the evaporative fraction retrieved by the triangle method.

The predictive performance of the different G -parameterisation schemes were assessed by means of the root mean square error (RMSE) and mean bias error (MBE) of the resulting retrieved values (H_r) with respect to the observed values (H_{obs}).

4.4. Performance assessment and discussion

4.4.1. Parameterisation of γ_{dry} and α_{dry}

▪ *Dry season*

The average values of surface parameters (α_{dry} , γ_{dry} , NDVI_{dry} , a_{dry}) and fluxes ($R_{n,\text{dry}}$, H_{dry} , G_{dry}) at the four sites in the dry season are presented in Table 3. The average values of α_{dry} and γ_{dry} , varied in the interval [0.19-0.28] and [0.28-0.40], respectively, the highest value being found for Eguerit, the less vegetated site, with an average value of G_{dry} of 127 W m^{-2} , i.e. approximately 25-30% higher than the values found for the other sites ($G \approx 100 \text{ W m}^{-2}$). The variability of α_{dry} and γ_{dry} was higher than that of NDVI and albedo, and the variability of G higher than that of H . The latter suggests that changes in R_n affected more G than H_s under dry conditions. The explanation might be that G depends mainly on T_s while H_s is driven by the surface-to-air temperature gradient, $T_s - T_a$, which is less sensitive than T_s to a change in R_n . Overall, the variation range and order of magnitude observed for α_{dry} , γ_{dry} and G were plausible.

▪ *Wet season*

In the wet season, the values of α_{wet} assuming $\gamma_{\text{wet}} = 0.30$ were found to vary in the interval [0.02-0.09] and EF_{wet} in the interval [0.68-0.94] (Table 4). As expected, the lowest values of H_{wet} and G_{wet} were observed at the Sudanian site (Bellefoungou) where the West African Monsoon is most intense, and at the Sahelian site of Kelma, subject to flooding. The highest values were observed at the Sahelian sites of Banizoumbou and Eguerit, where the Monsoon influence is substantially attenuated.

Table 3: Mean values of surface parameters (α_{dry} , γ_{dry} , $NDVI_{dry}$, a_{dry}) and fluxes ($R_{n,dry}$, H_{dry} , G_{dry}) at the four sites in the dry season. In parenthesis, standard deviation

Site	$\alpha_{\delta_{p\psi}}$	$\gamma_{\delta_{p\psi}}$	$NDVI_{dry}$	a_{dry}	$R_{n,dry}$ (W m ⁻²)	H_{dry} (W m ⁻²)	G_{dry} (W m ⁻²)	EF_{dry} (fixed)
Banizoumbou	0.24 (± 0.06)	0.31 (± 0.10)	0.16 (± 0.01)	0.37 (± 0.02)	407 (± 24)	321 (± 19)	97 (± 26)	0
Eguerit	0.25 (± 0.11)	0.36 (± 0.19)	0.11 (± 0.02)	0.23 (± 0.03)	485 (± 65)	359 (± 13)	127 (± 39)	0
Kelma	0.19 (± 0.04)	0.24 (± 0.06)	0.16 (± 0.03)	0.19 (± 0.03)	504 (± 16)	408 (± 19)	96 (± 23)	0
Bellefoungou	0.22 (± 0.12)	0.36 (± 0.23)	0.42 (± 0.05)	0.20 (± 0.03)	479 (± 43)	310 (± 22)	106 (± 29)	0.15

Table 4: Mean values of surface parameters (α_{wet} , γ_{wet} , $NDVI_{wet}$, a_{wet} , EF_{wet}) and fluxes ($R_{n,wet}$, H_{wet} , G_{wet}) at the four sites in the wet season. In parenthesis, standard deviation

Site	α_{wet}	γ_{wet} (fixed)	$NDVI_{wet}$	a_{wet}	$R_{n,wet}$ ($W\ m^{-2}$)	H_{wet} ($W\ m^{-2}$)	G_{wet} ($W\ m^{-2}$)	EF_{wet}
Banizoumbou	0.05 (± 0.01)	0.30	0.29 (± 0.01)	0.30 (± 0.02)	581 (± 23)	95 (± 27)	28 (± 84)	0.83 (± 0.04)
Eguerit	0.09 (± 0.02)	0.30	0.11 (± 0.02)	0.22 (± 0.02)	475 (± 110)	141 (± 48)	42 (± 14)	0.68 (± 0.07)
Kelma	0.02 (± 0.01)	0.30	0.56 (± 0.03)	0.09 (± 0.01)	802 (± 50)	49 (± 26)	15 (± 8)	0.94 (± 0.03)
Bellefoungou	0.07 (± 0.01)	0.30	0.58 (± 0.13)	0.15 (± 0.01)	689 (± 74)	162 (± 30)	49 (± 9)	0.75 (± 0.04)

4.4.2. Representation in the EF- α space

When plotted in the EF- α space, the seasonal mean values of α showed a clear decreasing trend with increasing EF (Figure 24). A linear regression was fitted to these mean values, yielding the following empirical relationship between the site-averaged values of α and EF obtained for the dry and the wet season ($R^2 = 0.96$):

$$\alpha = -0.22EF + 0.23 \quad (47)$$

Note that this relationship is close to the α - EF relationship provided by Eq. 41 or $\gamma = 0.30$ (Figure 23):

$$\alpha = \frac{0.3(1 - EF)}{1 + 0.3(1 - EF)} \quad (48)$$

In the following, Eq. 47 was used as the parameterisation formula linking α to EF

Figure 24: Relationship α vs EF. Points are average-site values of the dry and wet season (Table 3 and Table 4). The dashed line is the linear regression fitted to the points (Eq. 47). The thick line ($\gamma = 0.3$) is Eq. 48.

4.4.3. Relationship between α and surface attributes (NDVI, albedo)

Plotting the site-average values of α against the corresponding average NDVI values (Figure 25) revealed that there was no clear correlation between the two surface attributes. Rather, it was found a clear separation between the dry and wet seasons, with two clusters, one corresponding to high values of α and the other to low values. Therefore, α could not be accurately described over the whole range of EF when considering NDVI as the only explicative variable.

In the same figure, three formulae proposed in the literature are also shown:

- the linear function proposed by Su (2002):

$$\alpha = \alpha_0 + (\alpha_{\max} - \alpha_0)(1 - f_c) \quad (49)$$

where $\alpha_0 = 0.05$ and $\alpha_{\max} = 0.315$, f_c is the cover vegetation fraction computed as $f_c = (\text{NDVI} - \text{NDVI}_{\min})^2 / (\text{NDVI}_{\max} - \text{NDVI}_{\min})^2$, with $\text{NDVI}_{\min} = 0.08$ (observed at Eguerit) and $\text{NDVI}_{\max} = 0.86$ (observed at Bellefoungou).

- the formula of Bastiaanssen (2000)

$$\alpha = 0.20(1 - 0.96\text{NDVI}^4) \quad (50)$$

- the function proposed by Moran et al. (1994)

$$\alpha = 0.583 \exp(-2.13\text{NDVI}) \quad (51)$$

None of the above empirical formulae captured the annual changes in α , as shown by the two distinct clusters of points. Rather, it appears necessary to use two distinct equations for α , one for the dry season, and another one for the wet season.

Plotting the site-average values of α against the corresponding average albedo values (Figure 26) led to the same conclusion as that drawn for NDVI, that is, there was a clear separation between the dry and wet seasons that cannot be accounted for by a unique relationship between α and surface albedo.

Figure 25: Evolution of α vs NDVI for the dry (open squares) and wet season (black circles). The dashed line is the function proposed by Moran et al., 1994: $\alpha = 0.583 \exp(-2.13 \text{ NDVI})$, the cross-line is the formula of Bastiaanssen et al. (2000) $\alpha = 0.20 (1 - 0.96 \text{ NDVI}^4)$. The continuous curve is the function proposed by Su (2002): $\alpha = \alpha_0 + (\alpha_{\max} - \alpha_0) (1 - f_c)$ where $\alpha_0 = 0.05$ and $\alpha_{\max} = 0.315$. f_c being the cover vegetation fraction computed as $f_c = (\text{NDVI} - \text{NDVI}_{\min})^2 / (\text{NDVI}_{\max} - \text{NDVI}_{\min})^2$, with $\text{NDVI}_{\min} = 0.08$ (observed at Eguerit) and $\text{NDVI}_{\max} = 0.86$ (observed at Bellefougou).

Figure 26: Evolution of α vs albedo for the dry (open squares) and wet (black circles) season.

4.4.4. Performance assessment of the parameterization schemes

A total of 451 retrieved values of H from MODIS-Terra overflights throughout the years 2005-2007 at the four sites were used to assess the performance of the new parameterisation scheme combined to the triangle method. Our ground reference values were the observed values of H (H_{obs}) obtained from the flux-tower measurements. The values of retrieved sensible flux, H_r , were calculated by means of Eq. 46, using the observed values of R_n , $R_{n,\text{obs}}$. The calculations were performed for four different parameterizations of G :

- Par-1: G was estimated from the relationship α vs EF established in this study and given by Eq. 47
- Par-2; G was calculated following Su (2002), with α linked to the cover fraction, f_c , through Eq. 49
- Par-3: G was predicted from the formula proposed by Bastiaanssen (2000), (Eq. 50)
- Par-4: G was estimated from the formula proposed by Moran et al (1994), with α given by Eq. 51

The values of the statistical estimators RMSE and MBE of the relationship H_r vs H_{obs} (Table 5) indicated that there was a clear improvement of the predictions when using Par-1 for all sites, with respect to the VI-based parameterisation (Par-2 to Par-4). Among the latter, Par-3 was performing the best. Pooling the data of all sites, RMSE was 41.5 W m^{-2} and MBE was -11.2 W m^{-2} for Par-1, compared to 65.5 W m^{-2} and -51.3 W m^{-2} for Par-2, 50.4 and -25.1 W m^{-2} for Par-3 and 83.7 and -65.1 W m^{-2} for Par-4. To highlight the negative bias occurring in all the sites, the regression H_r vs H_{obs} using the best-performing parameterisation (Par-1) is presented in Figure 27 together with the regression lines. Underestimation of H occurred mainly in the upper range ($H > 300 \text{ W m}^{-2}$).

Table 5: Statistical estimators (RMSE and MBE, in $W\ m^{-2}$) of the regression analysis between H_r and H_{obs}

Site	Par-1 (Eq. 47)		Par-2 (Eq. 49)		Par-3 (Eq. 50)		Par-4 (Eq. 51)	
	RMSE	MBE	RMSE	MBE	RMSE	MBE	MBE	MBE
Banizoumbou	37.6	0.5	52.8	-37.7	41.2	-14.5	70.6	-47.3
Eguerit	41.3	-4.3	69.8	-58.3	47.9	-29.9	106.8	-58.3
Kelma	41.4	-33.9	86.6	-77.3	56.9	-51.5	105.3	-90.3
Bellefoungo	48.5	-22.4	70.8	-56	59.6	-42.5	62.7	-34.7
All sites	41.5	-11.2	65.5	-51.3	50.4	-25.1	83.7	-65.1

Figure 27: Comparison between retrieved (using Par-1) and observed sensible heat flux for (a) Banizoumbou (b) Eguerit (c) Kelma (d) Bellefoungou (e) all sites (pooled data). Dashed lines = linear regression, dotted lines = 1:1 relationship.

The H_r and ET_r mean relative difference of the VI-based formulae with respect to the EF-based formula highlighted a general underestimation of the VI-formulae (Table 6). The smallest differences with Par-1 were found for Par-3 (-10% and -8% respectively for H_r and ET_r). The reason for the relatively close agreement between Par-1 and Par-3 predictions could stay in that (i) Par-3 predicted similar values of α as Par-1 for the dry season (Figure 25) and (ii) differences in α for the wet season were not very critical when retrieving ET at high EF because of the small relative weight of the ground heat flux in the energy balance. This result underlined that a realistic estimation of the value of α in the dry season is one of the main requirements to get reliable values of the other terms of the energy balance in semi-arid regions.

Table 6: Mean values ($W m^{-2}$) of retrieved fluxes (G , H and ET) and relative mean differences (RMD, %) of VI-based values (Par-2, Par-3, Par-4) with respect to the values supplied by Par-1

	Par-1 (Eq. 47)	Par-2 (Eq. 49)		Par-3 (Eq. 50)		Par-4 (Eq. 51)	
	Mean	Mean	RMD	Mean	RMD	Mean	RMD
G	52.4	124.0	137%	90.9	74%	159.0	204%
H	217.1	176.3	-19%	199.1	-10%	166.4	-25%
ET	199.6	168.7	-19%	179.1	-8%	159	-26%

4.5. Discussion

4.5.1. Performance of the EF-based parameterisation

The statistical estimators RMSE and MBE obtained for Par-1 were about 40 Wm^{-2} and -10 Wm^{-2} , respectively, for sensible heat flux. This is an acceptable performance when compared with other retrieval methods. Kalma et al. (2008) performed a reanalysis of 30 published validations to estimate λE from remote sensing, and showed that the average RMSE was about 50 W/m^2 , ranging from 20 to 132 W/m^2 . The errors obtained in the current study were also similar to other validation studies using the triangle method carried out for different sites and satellites' sensors, such as Southern Great Plains in the US with AVHRR and MODIS (Jiang and Islam 2001; Batra et al. 2006) or Northern Senegal in Western Africa with MSG-SEVIRI sensor (Stisen et al. 2008). Our study therefore confirmed the general validity and reliability of this method (Jiang and Islam, 2001; Batra et al., 2006; Stisen et al., 2008), and its robustness.

However, the difficulty in 'guessing' the wet edge in absence of fully wet pixels may lead to large uncertainties. This appears to be the main limitation of the method under dry and arid climates, as highlighted in this study by the systematic underestimation of H - and therefore, overestimation of λE - under very dry conditions ($H > 300 \text{ W m}^{-2}$) and for all sites (Fig. 6). The underestimation was especially strong for Eguerit (Fig. 6b) where almost all the predicted values were underestimated, with some errors reaching -150 W/m^2 . Note that Eguerit is the driest and the less vegetated of the four sites, and that the triangle method is especially prone to significant errors in determining the wet edge of the LST-NDVI space in very dry areas lacking of 'wet' pixels. The highest deviations could therefore be attributed to the retrieval algorithm rather than to the parameterisation approach of the soil heat flux.

4.5.2. Advantages and limitations of the EF-based parameterisation

The parameterisation scheme proposed in this work has the important advantage of being simple to apply, to be parsimonious in input requirements and to be based on a robust hypothesis, the decrease of G and H with increasing EF (i.e. with increasing soil moisture and/or vegetation cover). The method could potentially be applied to any semi-arid area with contrasted dry and wet seasons. Another advantage of the EF-based parameterisation is that EF includes the effects of the prevailing weather conditions and soil moisture regime at satellite overpass, whereas vegetation indices are varying slowly, and cannot account for sudden changes in weather or in recent rainfalls that modify the soil water status. In other words, EF captures the effect of rapid changes in aerial environment and soil moisture while vegetation indices respond to these changes with a large delay. This is the main argument in favour of the EF-based parameterisation

Our results also indicated that the choice of a vegetation index (NDVI, f_c) as predictor of α is likely to be the main cause of the relatively poor performance of the VI-based formulae (Table 5). The reason is that VIs cannot account for the contrasted soil moisture regimes of the dry and wet seasons. A possible recommended option would be to use two distinct α -VI relationships, one for the dry season and the other one for the wet season.

It is recognised several limitations inherent to the choice of R_n as predictive variable. Santanello and Friedl (2003) and Murray and Verhoef (2007a,b), among others, pointed out that G vs R_n relationships cannot account for the dependency of G on soil moisture and ignore the asymmetry in the diurnal variation of G relative to R_n . With the new parameterisation, the first drawback was minimised as α was expressed as a function of EF, which implicitly accounts for soil moisture and evaporation. The second drawback - asymmetry between G and R_n - implies that the proposed parameterisation (e.g. Eq. 47 or 48) would be valid only at the overpass time of MODIS-Terra. Applying the same equation to other hours of the day might be hazardous, as a lag exists between G and H which peaks at different hours (Santanello and Friedl, 2003).

To elucidate this point, we calculated the values of α_{dry} at the four sites for each hour of the period from 9:00 to 15:00, in the same way we did for the Modis-Terra overpass time (section 4.3.1.). The results (Figure 28) showed that, during the dry season, the parameter α_{dry} decreased from a maximum in the early morning (09:00) towards lower values or even negative values in the mid-afternoon hours.

Figure 28: Values of α_{dry} for each hour of the period 9.00 to 15.00 h. Symbols: circles = Bellefongou; squares = Kelma; triangles = Eguerit; diamond = Bani. The curves are the best fit of Eq. 12 (SF-model) to the points.

The decreasing trend was well described by the empirical model proposed by Santanello and Friedl (2003), hereafter noted SF:

$$\alpha = A \cos \left[\frac{2\pi(t + 10800)}{B} \right] \quad (52)$$

where t is time of day in seconds ($t = 0$ at solar noon). The coefficients A (i.e., the maximum value of α) and B (indicative of the time lag between G and H) are adjusting factors which were set at 0.31 and 74,000 s respectively in the original SF-model. This relationship has been proven to provide improvement to estimated values of G (Chehbouni et al. 2008).

The SF- model adjustment was performed only for the dry season, for which α_{dry} could be determined with reasonable accuracy from the procedure described in section 4.3.1. For the wet season, the high uncertainty and relative errors on α_{wet} and its small range of variation prevent the same type of exercise.

We identified the best fit values of the parameters for the dry season (A_{dry} and B_{dry}) at the four sites, by minimising model RMSE (Table 7). The A_{dry} values ranged in the interval [0.24-0.35], with the lowest value found at the semi-tropical site (Bellefongou) and the highest value at the driest site (Eguerit). The coefficient B_{dry} varied in the interval [75000 - 96500], with the lowest value for Bellefongou and the highest value for Kelma

(acacia forest site). Both coefficients – especially A_{dry} - were well correlated with $NDVI_{dry}$ (Figure 29), and could be predicted by means of the following linear relationships:

$$A_{dry} = -0.31 NDVI_{dry} + 0.37 \quad R^2 = 0.86 \quad (53)$$

$$B_{dry} = -50900 NDVI_{dry} + 97160 \quad R^2 = 0.86 \quad (54)$$

The SF-model combined with Eqs. 53 and 54 supplied a fair prediction of α (Figure 29) and could be considered as a robust alternative to estimate α from NDVI when EF is very small (e.g., $EF < 0.1$).

Overall, the latter results reconciled partly the VI- and EF-based schemes. We demonstrated that the VI-based scheme could be applied for the dry season through a specific parameterisation of the SF-model. It is very likely that this parameterisation would not be valid for the whole year (see Figure 25) and that a specific parameterisation of the SF-model should be searched for the wet season. The latter suggests that surface moisture rather than VI is the primary factor that drives the annual trend of α . As the EF-scheme accounts for the surface moisture through EF, it can be applied over the whole year, independently of the season.

Table 7: Values of the parameters A_{dry} and B_{dry} (Eq. 52) and model RMSE at the four sites

Site	A_{dry}	B_{dry}	RMSE
Banizoumbou	0.29	86500	0.017
Eguerit	0.35	88000	0.028
Kelma	0.32	96500	0.017
Bellefoungou	0.24	75000	0.024

Figure 29: Relationship between observed (α_{obs}) and estimated (α_{est}) values of $\alpha = G/R_n$. Estimates from the SF-model with A_{dry} and B_{dry} given by Eqs. 53 and 54. The line is the linear regression $\alpha_{est} = 0.96 \alpha_{obs} + 0.01$ ($R^2 = 0.94$, $RMSE = 0.029$)

4.6. Conclusion

Our EF-based parameterisation scheme, applicable to the whole range of EF, appears more robust than other existing empirical methods as it implicitly includes the effect of soil moisture and soil properties. It also relies on a more solid theoretical basis as we established that α is functionally related to EF. Besides, it was demonstrated that, under dry surface conditions (lower range of EF), the diurnal asymmetry between G and R_n at each site could be accounted for by linking the coefficients of the SF-model to NDVI.

The two methods provide empirical but practical alternatives to the universal but more complex method based on solving the physically-based equations that describe the process of soil heat conduction through a harmonic analysis of surface temperature (Murray and Verhoef 2007a,b; Verhoef et al. 2012). The choice between the two approaches should be made in function of the available input data on physical properties and water status of the soil, keeping in mind that the empirical approach is much less demanding in input data and computational process than the physically-based approach.

Chapter 5: Comparative analysis of the triangle method and JULES estimates

5.1. Introduction

This chapter presents the results of a comparative analysis between latent heat flux (or evapotranspiration, ET) estimations retrieved with the RS-based triangle method and with the land surface model JULES. The comparisons were performed for the year 2004 for a gridbox of 1° located River Segura Basin in South-East Spain (shown in Figure 30). ET calculated with the triangle method was averaged over the area of that same 1° gridbox for the satellite overpass time (11AM).

First, a comparison between JULES with its default parameters and the triangle method is carried out. Next, a range of different input parameters are varied within Monte Carlo (MC) simulations to study the sensibility of JULES to these parameters, and to explore the possibility to use the MC-method as a calibration tool for JULES. Several set of runs with different variation intervals of selected model parameters are completed. Finally, advantages, limitations and recommendations regarding the proposed calibration method are discussed.

Throughout this chapter, the RS-based triangle method is assumed to provide more reliable estimations of ET than the non-calibrated JULES model, because the lack of information with respect to the input parameters limits highly the accuracy of the LSM.

Figure 30: 1° Gridbox considered in this chapter.

5.2. Comparison with JULES run with default parameters

JULES is first run with its default parameter values. The default values for plant phenology parameters and soil properties are showed in Table 8 and in Table 9 respectively. The land cover fraction used in the default run was the one provided by the land cover map produced by the MetOffice central ancillary file maker, and is shown in Table 10. Only the parameters that have been modified afterwards are shown here.

First, surface temperature predicted by JULES is compared to MODIS LST data (Figure 32). Predictions seem reasonable, although JULES appears to underestimate the surface temperature in spring and overestimate it on some days in summer.

Table 8: Default parameter values required by JULES for the standard vegetation surfaces.

Parameter	Broadleaf trees	Needleleaf trees	C3 grasses	C4 grasses	Shrubs
Canopy height (m)	19.01	16.38	0.79	1.26	1
Leaf area index	5	4	2	4	1
Minimum canopy capacity (kg m ⁻²)	0.5	0.5	0.5	0.5	0.5
Rate of change of canopy capacity with LAI (kg m ⁻²)	0.05	0.05	0.05	0.05	0.05
Ratio of the roughness length for heat to the roughness length for momentum	0.1	0.1	0.1	0.1	0.1
Infiltration enhancement factor	4	4	2	2	2
Root depth (m)	3	1	0.5	0.5	0.5
Lower temperature for photosynthesis (deg C)	0	-10	0	13	0
Upper temperature for photosynthesis (deg C)	36	26	36	45	36
Moisture availability below which leaves are dropped.	0.5	0.5	0.5	0.5	0.5

A phenology module has recently been introduced into JULES where leaf area index (LAI) is updated on a daily basis based on soil water content and temperature.

LAI can be transformed to NDVI (Normalised Difference Vegetation Index) through the relation of Gilabert et al. (1996):

$$NDVI = A - B \exp(-C LAI) \quad (55)$$

where A, B and C depend on the species.

In the following, our aim is to check whether JULES is able to reproduce the phenology seasonality captured by the satellite. As we are not focusing on the absolute value of NDVI, we choose $A = 1$, $B = 1$ and $C = 0.5$ for sake of simplicity.

Table 9: Default parameter values required by JULES for soil properties.

Parameter	Default value
soil albedo	0.11
Van Genuchten parameter $m = 1/(1-n)$	6.63
Van Genuchten parameter $1/\alpha$ (m^{-1})	0.049460
Hydraulic conductivity at saturation ($kg\ m^{-2}\ s^{-1}$)	0.004715
dry heat capacity ($J\ m^{-1}\ K^{-1}$)	1,185,676
dry thermal conductivity ($W\ m^{-1}\ K^{-1}$)	0.226873
Volumetric soil moisture content at the critical point (m^3 water per m^3 soil)	0.242433
Volumetric soil moisture content at saturation (m^3 water per m^3 soil)	0.4582150
Volumetric soil moisture content at the wilting point (m^3 water per m^3 soil)	0.136328

Table 10: Land cover fraction for the studied gridbox according to the land cover map produced by the MetOffice central ancillary file maker

	Bare soil	Broadleaf trees	Needleleaf trees	C3 grasses	C4 grasses	Shrubs
Land cover fraction	24.1%	2.9%	2.0%	44.6%	10.3%	16.0%

Figure 31: Comparison of land surface temperature estimated by JULES with LST product from MODIS.

In Figure 32, we compare the seasonality of NDVI-JULES with NDVI-MODIS. NDVI-JULES was estimated with two different options that the model offers: drought phenology “on” and “off”. With the “on” option, the model simulates the drying out and death of the plants beneath a given level of available water. With the “off” option, the plants simply stops to grow (photosynthesis set to zero) when no more water is available.

None of the two options is able to reproduce the real seasonality of the vegetation as provided by MODIS-NDVI (Figure 32). However, the drought phenology option has a relatively small impact on the output ET value (Figure 33), and cannot explain by itself the important differences observed between the LSM and the RS-based method. The RMSE calculated when ET estimated by JULES (from now on referred to as ET-JULES) is compared to ET estimated by the triangle method (from now on referred to as ET-Triangle) was 69.25 W m^{-2} when the drought phenology option was turned on, and 67.86 W m^{-2} when drought phenology option was turned off.

Figure 32: Comparison of NDVI estimated from JULES LAI (eq. 55) and MODIS NDVI product. The black dots are NDVI from MODIS. The red line is NDVI estimated by JULES with the drought phenology option on, and the blue line is NDVI estimated by JULES with the drought phenology option off.

Figure 33: Comparison of ET-JULES and ET-Triangle. ET is in ($W m^{-2}$). The black dots are ET-Triangle. The red line is ET-JULES with the drought phenology option on, and the green line is ET-JULES with the drought phenology option off.

There is a clear overestimation of ET-JULES in spring with respect to ET-Triangle, which is consistent with the observed under-estimation of LST-JULES for the same period (Figure 31). This overestimation of ET results in cooling down of the surface in the model. In spring, the surface is drying out quicker in the model than in reality, leaving no water in summer for the ET process, hence resulting in an under-estimation of ET during the

summer months. This, again, is consistent with the overestimation of LST by JULES with respect to MODIS-LST for the same period.

Logically, we can hypothesise that these large errors are caused by an incorrect parameterisation of surface resistance to ET. The modelled resistance is likely to be too low, resulting in too high values for ET in the spring months and in completely dry soil in the summer months. The overestimation of the surface resistance can be ascribed to the large uncertainties contained in several input parameters. In what follows we consider the ones that are thought to have the largest impact on ET estimation.

5.3. Calibration with Monte Carlo simulations

To identify the set of parameters to which JULES is most sensitive, we run MC simulations varying different sets of input parameters in JULES. MC simulations consist in repeating model runs changing randomly, within a plausible range, some of the input parameters whose value is associated with high uncertainty. The objective is to find realistic values of the input parameters when these are unknown (or known but with large uncertainties).

Four series of MC simulations are carried out, each of them with different sets of input parameters:

- Fraction of bare soil, and 5 Plant Functional Types (PFT) fractions are varying randomly.
- Varying phenology parameters: 10 parameters are varying randomly.
- Varying soil parameters: 9 parameters are varying randomly
- All the above mentioned are varying at the same time.

These parameters are selected because they are thought to be the ones that would have the most significant effect on ET. Given that the studied area is located in S-E Spain which has a semi-arid climate, the drought phenology option is chosen in all runs.

Hereafter, the adjective “best” (set of parameters) is associated to the simulation that minimises RMSE when ET-JULES is compared to ET-Triangle, but does not necessarily mean that it corresponds to the set of parameters whose values are the most realistic or closest to the reality.

5.3.1. Fractional cover

The first hypothesis we test is whether the large differences between JULES and the triangle method could be explained by an inadequate choice and distribution of land cover type within the studied gridbox.

The varying parameters are the fraction of bare soil, and the proportion of each PFTs (broadleaf tree, needleleaf tree, C3 grass, C4 grass and shrubs). The snow tile and urban tile are kept to zero. All the other parameters are set to their default value (phenology and soil properties parameters with values shown in Table 8 and Table 9 respectively). One thousand simulations were run. The simulations are run supposing that the land cover fraction is unknown, so that the fraction of each tile can vary within the range of 0 to 100% with the only condition that the sum of all tiles would be equal to 100%.

In Figure 34, the dots represents ET estimations provided by the triangle method, the grey-shaded area shows the range within which ET-JULES varies in that 1000-simulations, and the red line displays the “best” match of JULES, i.e. the run with the set of parameters that was closest to the estimations given by the triangle method over the year 2004 (lowest RMSE).

For this first set of simulations, the “best” simulation is achieved with the values of fractional cover presented in Table 11 (RMSE = 50.29 W m⁻²). This simulation still predicts ET-JULES-values that are too high in spring when compared to ET-Triangle, although the underestimations in summer are lower than those predicted by the default run.

The grey-shaded area in Figure 34 represents the uncertainty in ET-JULES associated with the uncertainty in land cover fraction. This area is quite large with an average uncertainty of 61 W m⁻² and a maximum uncertainty of 222 W m⁻². The average uncertainty ($\bar{U}$) and the maximum uncertainty (U_{max}) are defined as:

$$\bar{U} = \left(\sum_{i=1}^{366} (ET_{max,i}^{JULES} - ET_{min,i}^{JULES}) \right) / 366 \quad (56)$$

$$U_{max} = \max (ET_{max,i}^{JULES} - ET_{min,i}^{JULES})_{i=1}^{366} \quad (57)$$

where $ET_{\min,i}\text{-JULES}$ is the lowest simulated ET value for day i , and $ET_{\max,i}\text{-JULES}$ is the highest simulated ET value for day i .

Figure 34: ET-Triangle compared with one thousand simulations of JULES, varying fractional cover. ET is in ($W m^{-2}$). The black dots are ET-Triangle. The grey- shaded area corresponds to the range in which ET-JULES varies in those 1000 simulations. The red line represents the “best simulation” of JULES with the set of parameters that minimised the RMSE when compared with the triangle method.

To assess whether the retrieved proportion was realistic, we compared those values with a land cover map provided by MODIS MOD12Q1 Land cover product, classification type 3 (based on LAI/fPAR) for year 2004, shown in Figure 35. The percentage for each land cover type following this classification in our studied 1° gridbox is summarised in Table 12.

When comparing the land cover type defined in JULES with MODIS MOD12Q1 Land cover product (classification type 3), we have to take into account that the two classifications are defined in different ways, and therefore, they cannot be directly compared. Thus, in MODIS land cover types, for each non-vegetated class corresponds a bare soil percentage. This percentage is relatively low for forest (broadleaf or needleleaf) but is very high for shrubs and savannah, and somewhat intermediate for crops. Indeed, in the SRB, a Mediterranean region with semi-arid climate, large areas are suffering from

desertification process, and extended areas are only sparsely vegetated with shrubs, situation which exacerbates erosion problems. Baret et al. (1993) proposed a method to estimate a proxy for bare soil fraction (f_{soil}) as a function of LAI, based on Beer-Lambert law:

$$f_{soil} = e^{-\kappa LAI} \quad (58)$$

where κ is the extinction coefficient of solar radiation. If we consider $\kappa = 0.5$ and LAI for shrubs and savannah equal to 1, this would be equivalent of having 60% bare soil within “shrubs” and “savannah” classes in the MODIS classification, therefore, the total non-vegetated area would be close to 45% in MODIS classification.

Table 11: Values of the fractional cover that minimised the RMSE value when ET-JULES was compared with ET estimated by the triangle method.

	Bare soil	Broadleaf trees	Needleleaf trees	C3 grasses	C4 grasses	Shrubs
“Best” fraction	80.57 %	18.81 %	0.49 %	0.03 %	0.00 %	0.09 %

Figure 35: Land cover map from MODIS MOD12Q1 Land cover product, classification type 3 (based on LAI/fPAR) for year 2004.

Table 12: *Percentage of each land cover class of MODIS MOD12Q1 Land cover product, classification type 3 (based on LAI/fPAR), in the studied 1° gridbox for year 2004.*

	Water	Grasses /Cereal crops	Shrubs	Broad- leaf crops	Savan- nah	Broad- leaf forest	Needle- leaf forest	Non- vege- tated	Urban
% in gridbox area	0.8 %	16.3 %	71.9 %	3.3 %	4.9 %	0.0 %	0.8 %	0.5 %	1.3 %

Therefore, the comparison between the MODIS land cover product and the simulated land cover retrieved from the Monte Carlo simulations in JULES would agree on that the largest part of the studied area is bare soil. However, bare soil proportion in JULES's "best" simulation seems excessive and the minor elements of land cover type are not properly partitioned. For JULES's "best" land cover fraction, the second most important class is broadleaf tree, all the rest of the classes being negligible; whereas in MODIS land cover product, the second most important class is grasses/cereal crops.

JULES gridbox output is a weighted-average of the different tiles. Thus, the bare soil tile will have the highest influence in the estimated ET value; and the minor elements of the land cover will have a relatively small impact on the overall result. Although the "best" land cover fraction retrieved through the Monte Carlo simulations is able to improve slightly the results of ET-JULES, it cannot be considered an acceptable approximation of the real land cover (when compared to MODIS MOD12Q1 Land cover product). This suggests that the differences between ET-Triangle and ET-JULES are not due (or at least not entirely) to an inadequate distribution of land cover fraction, but rather to a wrong parameterisation of phenology factors and soil properties.

Note that neither the "best" land cover in JULES nor MODIS land cover product have values close to the default land cover provided by the land cover map produced by the MetOffice central ancillary file maker shown in Table 10 (page 110). This suggests that the reliability of the latter is limited, and that it is worth considering calibrating locally the land cover fraction when using JULES.

5.3.2. Phenology parameters

The second hypothesis we test is whether an inadequate assignation of phenology parameters values could be causing the differences between the triangle method and JULES. To that end, the following set of parameters related to plant phenology parameters is let to vary:

- *canht_ft*: canopy height (m)
- *lai*: leaf area index
- *catch0*: Minimum canopy capacity (kg m^{-2}). This is the minimum amount of water that can be held on the canopy.
- *dcatch_dlai*: Rate of change of canopy capacity with LAI (kg m^{-2}). Canopy capacity is calculated as $\text{catch0} + \text{dcatch_dlai} \cdot \text{lai}$.
- *dz0v_dh*: Rate of change of vegetation roughness length for momentum with height. Roughness length is calculated as $\text{dz0v_dh} \cdot \text{canht_ft}$.
- *infil_f*: Infiltration enhancement factor. The maximum infiltration rate defined by the soil parameters for the whole gridbox may be modified for each PFT to account for tile-dependent factors, such as macro-pores related to vegetation roots.
- *rootd_ft*: Root depth (m). An exponential distribution with depth is assumed, with e-folding depth *rootd_ft*. Note that this means that generally some of the roots exist at depths greater than *rootd_ft*.
- *Tlow*: Lower temperature for photosynthesis ($^{\circ}\text{C}$).
- *Tupp*: Upper temperature for photosynthesis ($^{\circ}\text{C}$).
- *fsmc_of*: Moisture availability below which leaves are dropped (parameter available when drought phenology is on).

Parameters *canht_ft*, *lai*, *rootd_ft*, *Tlow* and *Tupp* are varied individually for each PFT, whereas for the rest of parameters, the same value was applied for all the PFTs. The range for each phenology parameters is shown in the first column for each PFT in Table 13. The ranges are defined assuming that the real values are unknown, therefore the range is supposed to represent all the possible values that can be found in nature.

For this set of runs, the soil properties parameters and land cover fraction are kept unchanged and set to their default values (Table 9 and Table 10 respectively).

Table 13: Range within which phenology parameters were varied in the Monte Carlo simulations and values of the phenology parameters that minimised the RMSE value when ET JULES was compared with ET-Triangle (considered as the “best” set of parameters).

Parameter	Broadleaf trees		Needleleaf trees		C3 grasses		C4 grasses		Shrubs	
	Range	“Best”	Range	“Best”	Range	“Best”	Range	“Best”	Range	“Best”
canht_ft	2 - 20	9.77	2 - 20	16.11	0.2 - 1.5	1.41	0.2 - 2	1.32	0.2 - 2	1.77
lai	1 - 9	3.03	1 - 9	6.72	1 - 5	1.57	1 - 7	3.96	0.5 - 5	3.56
catch0	0 - 0.8	0.67	0 - 0.8	0.14	0 - 0.8	0.22	0 - 0.8	0.06	0 - 0.8	0.79
dcatch_dlai	0 - 0.2	0.17	0 - 0.2	0.06	0 - 0.2	0.19	0 - 0.2	0.12	0 - 0.2	0.02
dz0v_dh	0 - 0.5	0.152	0 - 0.5	0.28	0 - 0.5	0.43	0 - 0.5	0.32	0 - 0.5	0.21
infil_f	0 - 8	4.53	0 - 8	7.55	0 - 8	1.23	0 - 8	6.19	0 - 8	7.80
rootd_ft	2 - 10	9.99	0.5 - 5	1.10	0 - 2	1.93	0 - 2	1.03	0 - 2	1.46
Tlow	-10 - 10	-5.51	-20 - 0	-18.9	-10 - 10	-8.29	0 - 20	1.43	-10 - 10	-5.79
Tupp	25 - 45	38.86	20 - 40	29.04	20 - 45	38.8	35 - 55	36.03	25 - 45	32.18
Fsmc_of	0 - 0.8	0.23	0 - 0.8	0.35	0 - 0.8	0.75	0 - 0.8	0.76	0 - 0.8	0.44

The second column for each PFT in Table 13 shows the value of that parameter for the “best” set of parameters (the set of parameters that supplies the lowest RMSE when ET-JULES is compared to ET-Triangle). The RMSE for JULES run with the “best” set of parameters was 45.44 W m^{-2} .

As shown in Figure 36, this set of parameters does not allow reproducing the annual trend of ET provided by the triangle method. The main problem is still the overestimation of ET-JULES in spring.

The grey-shaded area in Figure 36 represents the uncertainty in ET-JULES associated with the uncertainty in the values of phenology parameters. This area is quite large, similar to the one observed for land cover fraction (Figure 34), with an average uncertainty (eq. 56) of 39 W m^{-2} and a maximum uncertainty (eq. 57) of 202 W m^{-2} .

Figure 36: *ET-Triangle compared with one thousand simulations of JULES, varying phenology parameters. ET is in ($W m^{-2}$). The black dots are ET-Triangle. The grey- shaded area corresponds to the range in which ET-JULES varies in those 1000 simulations. The red line represents the “best simulation” of JULES with the set of parameters that minimised the RMSE when compared with the triangle method.*

5.3.3. Soil properties parameters

The next hypothesis is whether inadequate values of soil properties parameters could explain better than the two previous sets of parameters the differences observed between the two approaches.

The soil properties parameters to be varied were the following:

- *albsoil*: soil albedo
- *m*: Parameters from the suction and hydraulic conductivity equations from van Genuchten (1980):

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha\Psi)^n]^m} \quad (59)$$

$$K_h = K_{hs} S^\xi \left[1 - (1 - S^{1/m})^m \right]^2 \quad (60)$$

where θ is the soil moisture concentration ($\text{m}^3 \text{ m}^{-3}$); θ_s is the soil moisture concentration at saturation ($\text{m}^3 \text{ m}^{-3}$); θ_r is the residual soil moisture concentration ($\text{m}^3 \text{ m}^{-3}$); α , n and m are the van Genuchten (1980) soil parameters, m being equal to $1-1/n$; Ψ is the soil suction (m); K_h is the hydraulic conductivity (m s^{-1}); K_{hs} is the hydraulic conductivity for saturated soil (m s^{-1}); and ξ is the snow insulation factor.

- *sathh*: $1/\alpha$ (m^{-1}), where α is a parameter of the van Genuchten model (van Genuchten, 1980) (see eq. 59)
- *satcon*: hydraulic conductivity at saturation ($\text{kg m}^{-2} \text{ s}^{-1}$)
- *hcap*: dry heat capacity ($\text{J m}^{-1} \text{ K}^{-1}$)
- *hcon*: dry thermal conductivity ($\text{W m}^{-1} \text{ K}^{-1}$)
- *sm_sat*: Volumetric soil moisture content at saturation (m^3 water per m^3 soil).
- *sm_crit*: Volumetric soil moisture content at the critical point (m^3 water per m^3 soil). The critical point is that at which soil moisture stress starts to restrict transpiration
- *sm_wilt*: Volumetric soil moisture content at the wilting point (m^3 water per m^3 soil).

The range of variation of these soil properties parameters is shown in the first column of Table 14. As in the above presented simulations, the range is defined assuming that no information about the real soil properties is known, and hence, the range is supposed to include all the possible values found in nature. The “best” set of parameters is

shown in the second column of Table 14. The RSME obtained for the run with this set of parameters is 31.3 W m^{-2} .

Table 14: Range within which soil properties parameters were varied in the Monte Carlo simulations and values of the soil parameters parameters that minimised the RMSE value when ET JULES was compared with ET-Triangle (considered as the “best” set of parameters).

Parameter	Range	“Best”
albsoil	0 - 0.6	0.59
m	5 - 10	5.28
sathh	0 - 3	2.54
satcon	0 - 0.5	0.43
hcap	100,000 - 2,000,000	1,385,005
hcon	0.15 - 7	0.32
sm_sat	0 - 1	0.55
sm_crit	0 - sm_sat	0.39
sm_wilt	0 - sm_crit	0.24

The uncertainty in ET-JULES associated with the uncertainty in the values of soil properties parameters (greyshaded area in Figure 37) is much larger than the uncertainty range observed with the two previous simulation runs. The average uncertainty (eq. 56) is 75 W m^{-2} and the maximum uncertainty (eq. 57) is 225 W m^{-2} . This result indicates that JULES is much more sensitive to changes in soil properties parameters than to changes in other model parameters. It can be drawn that special attention should be applied when defining the input values for these parameters. The default parameters in the case of this study appear to be inadequate for JULES to match the values calculated by the triangle method.

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Figure 37: ET-Triangle method compared with one thousand simulations of JULES, varying soil properties parameters. ET is in ($W\ m^{-2}$). The black dots are ET-Triangle. The grey- shaded area corresponds to the range in which ET-JULES varies in those 1000 simulations. The red line represents the “best simulation” of JULES with the set of parameters that minimised the RMSE when compared with the triangle method.

5.3.4. All parameters

When all the parameters mentioned in the previous paragraphs were allowed varying randomly and simultaneously, the lowest RMSE obtained was 29.1 W m^{-2} when compared with the triangle value (Figure 38). It is the lowest value achieved in all the experiments, representing a substantial improvement with regards to the initial run of JULES with its default values ($\text{RMSE} = 69.25 \text{ W m}^{-2}$). Comparison of the RMSE from the different experiments is shown in Table 15.

Figure 38: ET-Triangle compared with one thousand simulations of JULES, varying all the parameters presented in section 5.2.1. to section 5.2.3. ET is in (W m^{-2}). The black dots are ET-Triangle. The grey-shaded area corresponds to the range in which E- JULES varies in those 1000 simulations. The red line represents the “best simulation” of JULES with the set of parameters that minimised the RMSE when compared with the triangle method.

Table 15: Summary of the RMSE obtained in the different experiments.

Experiment	RMSE (W m^{-2})
JULES with default parameters (phenology OFF)	67.86
JULES with default parameters (phenology ON)	69.25
Monte Carlo simulations: "best" cover fractions	50.29
Monte Carlo simulations: "best" phenology parameters	45.44
Monte Carlo simulations: "best" soil properties parameters	31.30
Monte Carlo simulations: "best" parameters - ALL	29.10

The grey-shaded area in Figure 38 is larger than when the different sets of parameter is considered independently. This shows that the uncertainties have a cumulative effect and increase significantly when the number of unknown parameters is incremented. The average uncertainty (eq. 56) is 93 W m^{-2} and the maximum uncertainty (eq. 57) is 478 W m^{-2} . Table 19 shows the comparison of the uncertainties in the four experiments described.

This finding highlights the need to reduce the uncertainties on the value of the input parameters, in particular those that lead to large errors on the output values, like soil-related parameters. The maximum uncertainty (478 W m^{-2}) is extremely large, and 15% of the days of year 2004 have an uncertainty that exceeds 150 W m^{-2} (most of these days, in spring and summer). Thus, if the input parameters are inaccurately defined, the estimation of ET might be highly unrealistic.

The "best" parameter values are shown in bold in Table 16, Table 17 and Table 18. In those tables, results from the previous sections (sections 5.3.1. to 5.3.3.) and the default values (from section 5.2.) are also shown for sake of comparison. Note that:

- (i) In the current section, all the "best" parameters from the three tables when applied simultaneously provided the "best" JULES simulation (with lowest RMSE)
- (ii) In the previous sections, each table gives the set of "best" parameters for that specific group of parameters, while the rest of the parameters are set to the default values.

It can be seen that the default values and the “best” parameters in the different experiments have very different values. This suggests that different set of parameters can lead to similar results. Therefore high caution is required when interpreting the results because similar output might be obtained with distinct sets of input parameters. That is, the user should always verify that the input parameters are within a realistic range.

Table 16: Default values of the fractional cover, and values that minimised the RMSE value when ET JULES was compared with ET-Triangle for experiment 1 (section 5.3.1.) and experiment 4 (section 5.3.4.).

	Bare soil	Broadleaf trees	Needleleaf trees	C3 grasses	C4 grasses	Shrubs
Default	24.1%	2.9%	2.0%	44.6%	10.3%	16.0%
Experiment 1	80.57 %	18.81 %	0.49 %	0.03 %	0.00 %	0.09 %
Experiment 4	43.3 %	22.4 %	15.4 %	13.7 %	0.5 %	5.7 %

Table 17: Default values of the soil parameters, and values that minimised the RMSE value when ET JULES was compared with ET-Triangle for experiment 3 (section 5.3.3.) and experiment 4 (section 5.3.4.).

Parameter	Default value	Experiment 3	Experiment 4
albsoil	0.11	0.59	0.41
m	6.63	5.28	5.76
sathh	0.049460	2.54	2.31
satcon	0.004715	0.43	0.33
hcap	1,185,676	1,385,005	776,249
hcon	0.226873	0.32	1.40
sm_sat	0.242433	0.55	0.51
sm_crit	0.4582150	0.39	0.46
sm_wilt	0.136328	0.24	0.25

Table 18: Default values of the phenology parameters, and values that minimised the RMSE value when ET JULES was compared with ET-Triangle for experiment 2 (section 5.3.2.) and experiment 4 (section 5.3.4.).

Parameter	experiment	canht _ft	lai	catch _0	dcatch _h_ dlai	dz0v_ _dh	infil_f	rootd _ft	Tlow	Tupp	Fsmc_ _of
Broad- leaf trees	D	19.01	5	0.5	0.05	0.1	4	3	0	36	0.5
	2	9.77	3.03	0.67	0.17	0.152	4.53	9.99	-5.51	38.86	0.23
	4	12.4	3.08	0.7	0.11	0.5	4.73	8.27	-4.46	34.4	0.85
Needle- leaf trees	D	16.38	4	0.5	0.05	0.1	4	1	-10	26	0.5
	2	16.11	6.72	0.14	0.06	0.28	7.55	1.1	-18.9	29.04	0.35
	4	2.25	3.99	0.43	0.06	0.31	1.89	0.7	-15.4	26.8	0.65
C3 grasses	D	0.79	2	0.5	0.05	0.1	2	0.5	0	36	0.5
	2	1.41	1.57	0.22	0.19	0.43	1.23	1.93	-8.29	38.8	0.75
	4	1.45	1.65	0.58	0.01	0.03	1.62	1.23	-4.63	34.1	0.81
C4 grasses	D	1.26	4	0.5	0.05	0.1	2	0.5	13	45	0.5
	2	1.32	3.96	0.06	0.12	0.32	6.19	1.03	1.43	36.03	0.76
	4	1.68	5.73	0.16	0.09	0.08	2.25	1	15.1	48.1	0.51
Shrubs	D	1	1	0.5	0.05	0.1	2	0.5	0	36	0.5
	2	1.77	3.56	0.79	0.02	0.21	7.8	1.46	-5.79	32.18	0.44
	4	1.76	3.1	0.7	0.01	0.31	6.21	1.36	7.8	27.7	0.31

Table 19: For each experiment, value of the average annual uncertainty ($\bar{U}$, eq. 56) and the maximum uncertainty ($U_{\max}$, eq. 57).

Experiment	$\bar{U}$ (W m ⁻²)	$U_{\max}$ (W m ⁻²)
1	61	222
2	39	202
3	75	225
4	93	478

5.4. Sensitivity analysis

As shown in Section 5.3.3., JULES appears to be especially sensitive to soil-related input parameters. The aim of this section is to identify within the soil properties parameters, the ones that have the major impact on JULES output. To that end, additional Monte Carlo runs are carried out, by varying a single soil parameter at a time. The results are given in Figure 39 to Figure 46.

The main conclusion of these runs is that each parameter separately has a relatively small effect on the output, but the cumulative effect of all parameters changing together seems to have a noticeable impact on the estimations (Figure 37). Nevertheless, we can still identify some parameters that have a higher impact on the result, such as the soil albedo *albsoil* (Figure 39), the soil moisture at critical point *sm_crit* (Figure 44) and the soil moisture at the wilting point *sm_wilt* (Figure 46), which display larger range of variation of ET-JULES (grey-shaded area).

Figure 39: Monte Carlo runs for parameter *albsoil*

Figure 40: Monte Carlo runs for parameter *m*

Figure 41: Monte Carlo runs for parameter hcon

Figure 44: Monte Carlo runs for parameter sm_crit

Figure 42: Monte Carlo runs for parameter satcon

Figure 45: Monte Carlo runs for parameter sm_sat

Figure 43: Monte Carlo runs for parameter sathh

Figure 46: Monte Carlo runs for parameter sm_wilt

Figure 47: Monte Carlo runs for parameter sm_sat , sm_crit and sm_wilt changed jointly

A set of runs where the three soil moisture parameters (soil moisture at critical point, soil moisture at the wilting point and saturated soil moisture) are varied jointly (Figure 47) shows that JULES is particularly sensitive to those parameters.

The “best” parameter value for each set of Monte Carlo run is shown in Table 20 together with the RMSE value for each experiment. Note that:

- (i) In Table 14, all the “best” soil properties parameters when applied simultaneously provide the “best” JULES simulation (lowest RMSE).
- (ii) In Table 20, each parameter is varied individually to retrieve the “best” JULES simulation, while the rest of the parameters is set to the default values.

The parameters that induce the most significant reduction of the RMSE value are the same that show the largest range of variation of ET-JULES ($albsoil$, sm_crit , sm_wilt and sm_sat , sm_crit and sm_wilt varied jointly), and represent the parameters for which JULES is the most sensitive. These parameters show the highest values of average annual uncertainty ($\bar{U}$, eq. 56) and maximum uncertainty (U_{max} , eq. 57). Table 21 gives the value of $\bar{U}$ and U_{max} for all the soil properties parameters.

In particular, for sm_crit , the “best” value is very close to the default value. However, the RMSE is significantly lower for the simulation with the “best” value compared to the default run. This illustrates how small uncertainties in some input parameters can lead to large errors in the output estimation. In other words, JULES is highly sensitive to those parameters.

Some of “best” parameter values do not seem realistic. For example, the “best” soil albedo value is 0.6. In the RSB, a relatively high albedo value could be expected because of the arid character of the studied area with important extensions of dry and bare soil. However, a value of 0.6 is unrealistic, as even in deserts, soil albedo does not exceed values of 0.4. The “best” albedo value is also high when all the soil parameters are varying simultaneously (experiment 3, Table17), but is more realistic when all the parameters (phenology, cover fraction and soil properties) are varying simultaneously (experiment 4, Table17). This suggests that, in order to retrieve realistic values of input parameters, all the input parameters should be considered simultaneously. Otherwise, the error due to a wrongly assigned value of another parameter can have repercussions on the adjusted value of a given parameter.

Some of the parameters such as m (Figure 40), $hcon$ (Figure 41), $satcon$ (Figure 42) or $sathh$ (Figure 43) do not have a high impact on JULES output, even if they vary within a relatively wide range (Table 14, page 122). JULES is not very sensitive to these parameters, and hence, the uncertainty associated to these input values are not problematic.

Table 20: Default values of the soil parameters, and values that minimised the RMSE of ET-JULES compared with ET-Triangle, when varied individually, and their respective RMSE values.

Parameter	Default value	“Best”	RMSE (W m ⁻²)
<i>albsoil</i>	0.11	0.6	55.81
<i>m</i>	6.63	9.94	64.69
<i>sathh</i>	0.049460	0.0032	64.15
<i>satcon</i>	0.004715	0.0038	64.77
<i>hcap</i>	1,185,676	1,999,933	63.98
<i>hcon</i>	0.226873	6.99	62.00
<i>sm_sat</i>	0.242433	0.26	59.41
<i>sm_crit</i>	0.4582150	0.44	54.82
<i>sm_wilt</i>	0.136328	0.27	58.24
jointly { <i>sm_sat</i> <i>sm_crit</i> <i>sm_wilt</i>	0.4582150 0.242433 0.136328	0.74 0.65 0.55	52.4

Table 21: For each parameter, value of the average annual uncertainty ($\bar{U}$, eq. 56) and the maximum uncertainty ($U_{\max}$, eq. 57)

Parameter	$\bar{U}$ (W m ⁻²)	$U_{\max}$ (W m ⁻²)
<i>albsoil</i>	19	116
<i>m</i>	1.5	18
<i>sathh</i>	6	45
<i>satcon</i>	5	43
<i>hcap</i>	5.5	33
<i>hcon</i>	12.5	106
<i>sm_sat</i>	17.5	98
<i>sm_crit</i>	22	120
<i>sm_wilt</i>	28	132
jointly { <i>sm_sat</i> <i>sm_crit</i> <i>sm_wilt</i>	35	210

5.5. Discussion

The high grade of uncertainty in the numerous input parameters necessary to run LSM JULES makes its use in practice very difficult, unless the model parameters are calibrated locally. Using Monte Carlo simulations to try to adjust the model output to the values retrieved by a validated RS-based model is one possible option to achieve this calibration. Based on the results described in the previous sections of this chapter, the advantages and limitations of this proposed method are discussed in this section; and recommendations are formulated for the potential use of this calibration method.

5.5.1. Advantages of the proposed calibration method

The calibrated model, when all parameters were considered simultaneously, performed significantly better than the uncalibrated model (RMSE 29.10 W m^{-2} against 69.25 W m^{-2}). The calibrated model is able to eliminate the overestimation of ET in spring and underestimation of ET in summer that are observed in the default run (section 5.2.), and deliver more realistic estimations of ET over the year 2004.

When no actual information is available to accurately define the input parameters, this method is a valuable option to constrain the error of the model. If the input parameters values are completely unknown, the model could potentially give any value, but if the model is calibrated against a validated RS-based model estimations, the model with the adjusted parameters will provide a result closer to reality, within the accuracy of the RS-based model.

This method also allows combining the strengths of both method (LSM and RS-based model) to overcome their respective weaknesses. The RS-based method has the main advantage of been more reliable because it is based on observations and is validated, and it does not rely on the knowledge of numerous parameters. In addition, the triangle method has the great advantage of being constrained by the wet and dry limits, which avoid the retrieval of unrealistic value of ET. However, one of its main limitations is that it is discontinuous in time, as it only simulates ET once per day (at the satellite overpass time) and only for cloud free days. On the contrary, JULES provides a continuous hourly estimation, but is unreliable unless calibrated, because of the large number of input parameters necessary for its execution. When JULES is calibrated against the triangle

method, it combines the reliability of the latter with the continuity of the first. Time series of ET-Triangle can be gap-filled with JULES with this method, or future predictions can be retrieved with the calibrated LSM forced with the right driving data.

5.5.2. Limitations of the proposed calibration method

However, this method also suffers from several deficiencies that one has to bear in mind when applying it. First of all, because the calibration of one model is done against another model, this method will not be as accurate as a calibration done against *in situ* measurements. In the proposed calibration method, the values against which the LSM is being calibrated already include implicitly an error, which in the case of the triangle method, is estimated to be around 40 W m^{-2} (see chapter 4, Table 5).

Another important point to take into consideration is that there are an infinite number of combinations of parameters (because the ranges within which they vary are continuous). However, we only simulated 1000 cases for each experiment. This means that the “best” set of parameters is only the “best” among those 1000 cases, but might not be the real best set of parameters, as the latter might not be among the 1000 random cases simulated. Moreover, the parameters are varied randomly in the Monte Carlo simulations, which implies that the result is not reproducible, because if the experiment is repeated, the 1000 new combinations will be different from the previous ones. Nevertheless, we believe that 1000 cases produce a range wide enough to get reasonably close to the real best set of parameters, and we can consider it a compromise between accuracy and computational time.

Further critics of the method can be formulated regarding the possibility that the differences observed between ET with uncalibrated JULES and ET-Triangle might be induced by different causes than the ones considered in this study. Here, we based our comparative analysis on the hypothesis that the uncertainties in certain input parameters were responsible for the bias observed. However, one could argue that this bias might be caused by other reasons, among them:

- The driving data used to force JULES might not be reliable for the studied area. LSMs rely on trustworthy forcing data. However, the Princeton driving data used in this study is a complex product constructed by combining a suite of global observation-based datasets with the National Centers for Environmental

Prediction–National Center for Atmospheric Research (NCEP–NCAR) reanalysis (Sheffield et al., 2006). Corrections are made to adjust known biases, but the true accuracy of the dataset for the studied area is unknown.

- In JULES, some modules have different alternatives from which the user can choose from. For example, to calculate the soil hydraulic characteristics, the user has the choice between using Brooks and Corey (1964) equations or formulas proposed by Van Genuchten (1980). For surface runoff simulations, the user can chose from TOPMODEL (Beven and Kirkby 1979) or the Probability Distribution Model (PDM, Moore 1985). Other options apply to the choice of canopy model, photosynthesis model, stomatal conductance, vegetation dynamics, scaling up from plant to canopy, and others, which exhaustive description can be found in Best et al. (2011) and Clark et al. (2011). Consequently, part of the error observed in JULES initial run might be caused by the wrong combination of options, and could simply be improved by a different choice in some of the modules. Alton et al. (2007) showed that the choice of different representations of canopy photosynthesis and stomatal conductance options in JULES could lead to uncertainties of up to 60% for surface fluxes. This suggests that part of the error committed is due to an inaccurate description of the physics within the model rather than just a problem of adjusting the input parameters.
- The differences might be caused by parameters other than the ones considered in this study. In our set of experiments, we focused on a limited number of parameters that were thought to have a direct impact on ET. Nonetheless, there might be other parameters that significantly impact on ET estimation but that have not be considered in this study. Previous works, like Alton et al. (2007), have demonstrated the sensibility of ET-JULES to other parameters such as the light limited quantum efficiency, the rubisco limited rate of photosynthesis at the top of canopy and the near-infrared transmittance of vegetation, leading to uncertainties of up to 35% in surface fluxes.

Considering the above comments, we should be aware of the possibility that the calibrated model might provide the “right” answer, but under “wrong” assumptions. For example, in Section 5.4., we point out that the “best” value of soil albedo is unrealistic, being too high to represent a real soil. However, this unrealistic value of albedo is able to provide an improved estimation of ET. The overestimated albedo results in a reduction of net radiation, which in turn results in lower values of ET in spring (thus eliminating the overestimation of ET in spring). Consequently, less water is available for evaporation

during the summer months, hence eliminating the underestimation of ET in summer. As shown here, the “wrong” value of albedo enables the model to produce “right” values of ET. This is just an example to illustrate that the “best” set of parameters might not be representative of the reality, although it does improve the model performance.

Another point worth mentioning is that in this study, JULES has been calibrated against ET values, but the rest of JULES simulated output variables has not been considered. Therefore, the performance of calibrated JULES in simulating those other output parameters should also be analysed.

5.5.3. Recommendations

Extreme caution should be adopted in interpreting the results when the proposed calibration method is applied. One should keep in mind that getting the “best” ET estimation with a given set of parameters does not necessarily imply that these values are representative of the reality. Therefore, whenever possible, we would recommend using field values to adjust the input parameters, especially when defining the parameters to which JULES is the most sensitive to, such as soil moisture at the critical point, soil moisture at wilting point and soil albedo (see section 5.4.).

When there is a lack of field information, but the knowledge of the studied area is precise enough to derive reasonable proxies of the local properties, the proposed method could be recommended, adjusting the variation range of each parameter as narrowly as possible.

In any case, the MC method is still valid when no other information is available, and will generally provide better estimations than the default version.

5.6. Conclusion

This chapter had the double objective of (i) studying the sensibility of JULES to certain input parameters through Monte Carlo simulations, and (ii) assessing this method as a calibration tool using RS data to adjust the input parameters. We show that JULES is especially sensitive to soil-related parameters and, within this category, soil albedo, soil moisture at the critical point and soil moisture at wilting point are the parameters which induced the highest uncertainties in the retrieval of ET.

We conclude that the Monte Carlo method is a useful tool to undertake a comprehensive sensitivity analysis, but suffers from several limitations when used as a calibration tool to adjust LSM parameters. The main limitation is that the MC-method does not offer sufficient guaranty that the adjusted parameters are realistic values, as the solution might correspond to a local minimum. However, when no information is available to assign realistic values to the input parameters, this method can help improving the performance of the LSM, provided caution is applied to ensure that the parameters values are within a realistic range.

Chapter 6: Operational applications

6.1. Introduction

The objective of this Chapter is to illustrate the potential of RS-based tools to monitor surface fluxes in arid countries, with the presentation of three operational applications.

The first application is the use of the ET-retrieval triangle method as described in Chapter 4 for ET-mapping in West Africa regions influenced by the African Monsoon. The second one is the application of the triangle method to a long-time series (12 years) of MODIS images to generate a land surface climatology for the Segura River Basin (SRB). The third operational application is the use of sea surface temperature (SST) provided by MODIS-Aqua sensor to validate a mathematical model of water balance for a coastal lagoon in the SRB.

6.2. ET-mapping in regions under the influence of West African monsoon

Figure 49 to Figure 51 display the spatial and temporal evolution of ET in 3 areas in Central and Western Africa. The situation and extension of the studied areas are represented on the map of Figure 48. These are 170 km x 170 km areas with pixel size of 1 km x 1 km.

Figure 48: Studied area for ET-mapping.

Representative days of the dry and wet seasons were chosen to illustrate the differences that can be observed between these two periods. At the top of each figure (Figure 49a, Figure 50a, Figure 51a), a precipitation histogram is shown to help identifying the selected days within the temporal scale. These precipitations were registered at meteorological stations, and might not be representative of the whole area as the spatial variability of precipitation can be important, with highly localized storms.

Usually, cloud free satellite images during the monsoon period are very scarce. For some of the studied sites, not more than a couple of usable days were found during the whole rainy season.

The first general observation that can be made after examining Figure 49 to Figure 51 is that a clear drying out of the surface can be observed during the dry season with lower ET values, followed by an increase in ET during the wet season when there is more water available.

The maps illustrate the high sensibility of ET to water availability, and therefore justifies the use of ET as one possible approach to monitor drought in a region, usually as a ratio, either of actual ET and potential ET (ET/ET_p), such as in the Crop Water Stress Index CWSI (Jackson et al. 1981), or actual ET and available energy ($EF = ET/R_n$) (Nishida et al. 2003).

A spatial gradient of ET can be observed from south (greater ET) to north (lower ET), both inside the different studied areas, and between these (greater ET values in Benin than in Mali). These differences are explained by a gradient in rainfall, with much higher precipitations in the South, subject to oceanic influence, than in the north. This suggests that in these areas, ET is water-limited rather than radiation-limited.

These ET-maps illustrate the great potential of RS-based method to characterise spatiotemporal evolution of surface fluxes, and to help identifying areas prone to suffer from drought.

Figure 49: (a) Precipitation histogram for Baniboumzou (Niger) and (b) Evolution of ET, studied area in Niger. Map A corresponds to the end of the wet season (September 2006), Maps B to F correspond to the dry season (October 2006 to April 2007), Map G corresponds to the beginning of the wet season (May 2007), Maps H and I correspond to the wet season (June to September 2007), Map J corresponds to the end of the wet season (October 2007) and Map K corresponds to the dry season (November 2007).

Figure 50: (a) Precipitation histogram for Hedgerit (Mali) and (b) Evolution of ET, studied area in Mali. Map A corresponds to the end of the dry season (April 2005), Maps B to E correspond to the wet season (May 2005 to September 2005), and Maps G to K correspond dry season (October 2005 to May 2006).

(a)

(b)

Figure 51: (a) Precipitation histogram for Belifoungou (Benin) and (b) Evolution of ET, studied area in Benin. Maps A to C correspond to the dry season (December 2005 to February 2006), Maps D to G correspond to the wet season (Junes 2006 to October 2006), and Maps H to K correspond dry season (November 2006 to March 2007).

6.3. Land Surface Climatology from EO-Satellite Information (Segura River Basin)

6.3.1. Introduction

Land surface (or skin) temperature observations (LST) obtained by satellite remote sensing, and derived surface fluxes from retrieval algorithms provide useful climatological information of high spatial resolution and global coverage that enhances the traditional ground based observations at 2m and so, reveal new information about land surface characteristics and their response to land use modification, drought events or other mean to long term changes in land use and climate.

Several ET-retrieval methods (see section 2.2.2.) are available to estimate land evapotranspiration (ET) by satellite remote sensing. Such estimates are especially valuable as they provide spatial coverage of this important flux over large areas, but also because they allow building a long-term climatological data-set that complements that derived from flux-tower stations that monitor the energy and hydrologic balance at the land surface (e.g. Fluxnet).

This sub-chapter presents 12 years (2000-2011) of moderate-resolution imaging spectroradiometer (MODIS) LST observations to analyse monthly and inter-annual variations of the components of the surface energy balance (SEB) at three sites of the Segura River Basin (see description in section 3.2.2.). Changes in the SEB components are related to other MODIS-retrieved variables (LST, vegetation indices, albedo) in an effort to understand the physical mechanisms responsible for the changes in energy partitioning at the land surface. Of paramount importance in this study are the estimates of the evaporative fraction, EF, provided by the triangle algorithm (Chapter 4).

6.3.2. Data set and calculations*Evaporative fraction*

Windows of 267 km x 227 km integrating the pixels (1 km²) corresponding to the three sites were used to derive the evaporative fraction EF by means of the triangle method.

Net radiation

To calculate surface net radiation, ground hourly data of solar radiation (S), air temperature (T_a) and air humidity (e_a , partial vapour pressure) at 2m provided by the automatic weather stations located at each pixel, associated with the instantaneous values of LST (T_s) and albedo (a) obtained from the MODIS products.

The calculation steps for R_n were the following:

(i) Short-wave net radiation:

$$S_n = (1 - a)S \quad (61)$$

(ii) Long wave net radiation

$$L_n = L_d - L_{up} \quad (62)$$

with L_{up} = upward long wave radiation, = $\epsilon_s \sigma T_s^4$; and L_d = downward long wave radiation, that was calculated as proposed by Allen et al. (1998) from the air temperature T_a and water vapour pressure e_a at 2m.

(iii) Net radiation:

$$R_n = S_n + L_n \quad (63)$$

Ground heat flux, G

The ground heat flux G was calculated as proposed by Tanguy et al. (2012), using a relationship of the type $G = \alpha R_n$, where α is an empirical function of the evaporative fraction (Chapter 4, eq. 47): $\alpha = -0.22 + 0.23 \text{ EF}$

Evapotranspiration and sensible heat flux

ET was calculated as:

$$ET = EF \times (R_n - G) \quad (64)$$

and H as:

$$H = (R_n - G) - ET \quad (65)$$

Monthly mean values of the abovementioned variables were calculated for each month of the observation period. Missing monthly values for a variable were replaced by the average of the variable over the whole period. The average of the monthly values over the period 2000-2012 was determined for each month, providing the “average” year over the 12-year period for all the considered variables. Finally, the yearly average for the 12 years of the period was calculated, together with the yearly sum of precipitation, P (mm year⁻¹).

6.3.3. Time series of EF, LST and SEB components (2000-2011)

6.3.3.1. EF and LST

The Murcia's site presents generally the highest values of monthly EF, mainly during the summer months, followed by Calasparra and Jumilla (Figure 52). The latter site exhibits the highest LST whereas Murcia and Calasparra exhibit very similar LST pattern and values (Figure 53). Note that for the winter period, EF and LST are relatively similar at the three sites.

Figure 52: Evolution of monthly-evaporative fraction (EF) at MODIS-Terra overpass time at the three sites. Period 2000-2011

Figure 53: Evolution of monthly LST (T_s) at MODIS-Terra overpass time at the three sites. Period 2000-2011

6.3.3.2. SEB components

Figures 54 to 57 show the evolution of the monthly average of the components of the surface energy balance (ET , H , G and $R_n - G$ respectively) at the three sites. All the components present a cyclic trend with annual maximum and minimum values. The available energy, $R_n - G$, was significantly lower at Jumilla, which presents the highest albedo and surface temperature (Figure 53), and the lowest evapotranspiration rate among the three sites. The latter could be ascribed to two causes:

- Jumilla is the driest site (annual mean rainfall over 2000-2011 ≈ 265 mm against ≈ 335 mm at the two other sites)
- The Jumilla's pixel under study has no irrigated fields

Figure 54: Evolution of monthly-average evapotranspiration (ET) at MODIS-Terra overpass time at the three sites. Period 2000-2011

Figure 55: Evolution of monthly-averaged sensible heat flux (H) at MODIS-Terra overpass time at the three sites. Period 2000-2011

Figure 56: Evolution of monthly-averaged ground heat flux (G) at MODIS-Terra overpass time at the three sites. Period 2000-2011

Figure 57: Evolution of monthly-averaged available energy ($R_n - G$) at MODIS-Terra overpass time at the three sites. Period 2000-2011

6.3.4. Average year

6.3.4.1. NDVI

The three sites differed significantly among them in what refers to vegetation cover and its annual trend (Figure 58). The fully agricultural site, Calasparra, has its maximum NDVI in summer while Murcia and Jumilla have a parallel evolution, present the maximum NDVI in winter. Jumilla has the lowest NDVI throughout the year.

Figure 58: Annual trend of monthly values averaged over the 12-year period of (a) NDVI at the three sites. Bars = standard deviation (shown for Jumilla only)

6.3.4.2. EF and ET

The site of Murcia presents the highest values of EF (Figure 59a) and, consequently of ET (Figure 59b) in summer (months of June, July and August), due to the intensive irrigation of fruit trees during this period, while the sites of Calasparra and Jumilla, with practically no irrigated crops, present a maximum of EF and ET during the fall season (Sept. to Dec.), which corresponds to the period with the highest probability and amount of rainfall in the Segura River Basin. The differences between sites are more marked for ET between Jumilla and the two other sites because the available energy is substantially lower at Jumilla, the driest site (Figure 57).

The annual amplitude of EF differs among sites, confirming the effect of the significantly lower annual rainfall at the driest site (Jumilla), and an effect of intensively

irrigated agriculture at the Murcia site, possibly coupled to local advection effects during the warm season.

Figure 59: Annual trend of monthly values averaged over the 12-year period of (a) ET and (b) ET at the three sites. Standard deviations are typically 20-30 W m⁻².

6.3.4.3. Surface-to-air temperature difference ($LST - T_a$) and air VPD

The annual trend of the surface-to-air temperature difference, $LST - T_a$ (Figure 60a) confirms that Jumilla is the driest site, with monthly differences that reached 10°C on average in the months with the highest radiation (June and July), while the differences were substantially lower at Calasparra and Murcia.

The air vapour pressure deficit shows a similar annual trend to that of $LST - T_a$, (Figure 60b), but with less marked differences among sites. The increase rate of VPD_a is also slower than that of $LST - T_a$ at the start of the year, when radiation increases. It might be drawn that the surface-to-air temperature difference would be an earliest and more sensitive indicator than VPD_a for drought early warning.

Figure 60: Annual trend of monthly values averaged over the 12-year period of (a) the surface-to-air temperature difference, $LST - T_a$ and (b) air vapour pressure deficit (VPD_a) at the three sites.

6.3.5. Conclusion

Notwithstanding the uncertainties and errors associated with RS information and ET-retrieval methods, our attempt to build a climatology of RS-observed (e.g. LST) or RS-retrieved (e.g. EF) land surface attributes is encouraging. In particular, the results presented in form of average year appear coherent, enabling to describe and quantify the impact of the main drivers (rainfall, irrigation, type of surface and land use) that determine the annual trend of variables such as EF, of paramount importance for establishing the hydrological balance or assessing the impact of climate change and human activities on water resources.

However, other types of statistical treatments should be carried out with caution, as the number of observations could be highly variable in function of the period of the year. This is the case of LST, for which much more data are collected in summer than in winter. Such a characteristic of LST-data sets is likely to introduce a strong bias, for instance in the determination of histograms or cumulated frequency distribution (CFD) functions of LST, and therefore of EF. Maybe a solution would be to reconstruct continuous series of LST and EF using gap-filling techniques, or assimilating RS-data into LSM (Chapter 5).

6.4. Surface Energy Balance of water bodies (Mar Menor Lagoon)

The objective of the work described in this section was to analyse daily energy exchange of a coastal lagoon in S-E Spain (Mar Menor) with the atmosphere and with the adjacent Mediterranean Sea. To that end, a mathematical model to solve the energy balance of the lagoon was proposed. RS data was used as a validation tool to assess the performance of the model.

6.4.1. Description of the numerical model

Free-surface evaporation is mainly driven by the vapour pressure gradient between the water surface (at temperature T_s) and the nearby surrounding air (at temperature T_a). This implies that the knowledge of T_s is a prerequisite for the calculation of the evaporation rate. The first step was to include in the modelling approach the dynamic daily energy balance assuming steady state conditions during the 1-day period. This model predicts T_s using daily averaged climate data and the geometric characteristics of the water body (surface and depth) as input data. In the case of hypersaline coastal lagoons, the effects on the energy balance of water salinity and water exchanges with the sea must be taken into account in order to accurately predict the evaporation. Thus, the second step was to set and solve the salt and water balances simultaneously with the energy balance in order to obtain T_s at a daily scale. All outputs of the model are daily averaged values. The modelling approach was solved by means of an iterative numerical scheme. The equations are given below.

❖ Surface Energy Balance

The energy balance model was based on the fundamental laws of physics for energy and mass exchange, following the approach used by Losordo and Piedrahita (1991), Jacobs et al. (1997) and Martínez-Alvarez et al. (2007). Initial and boundary conditions were adapted to the special case of a coastal lagoon. In particular, it was assumed that thermal stratification was negligible (i.e. $T_s = T_w$) and that the following fluxes can be disregarded due to their minor importance in the energy balance (Henderson-Sellers 1986): 1) Energy losses by convection and conduction through the lagoon's bed, 2) Advective energy fluxes due to precipitation and runoff or groundwater discharges, and 3) Energy fluxes resulting from biological and chemical reactions.

With these assumptions, the energy balance at a daily time step was expressed as:

$$R_n + H_s + \lambda E + Q_{Med} = \Delta Q_w \quad (66)$$

where all fluxes are in $\text{MJ m}^{-2} \text{ d}^{-1}$. R_n is the net radiation of the water surface, H_s is the sensible heat exchanged between the air and the water surface, Q_{Med} is the energy exchanged with the Mediterranean Sea, ΔQ_w is the variation of energy in the water body occurring during the time interval, λE is the evaporation flux density from the surface, with E in $\text{kg m}^{-2} \text{ d}^{-1}$ ($= \text{mm d}^{-1}$) and λ is the latent heat of vaporization ($= 2.45 \text{ MJ kg}^{-1}$). All the fluxes have positive values when they represent heat inputs to the lagoon, and negative values when heat is lost. ΔQ_w is negative when energy is released and hence available for evaporation and positive when stored within the water column.

R_n was calculated using Equation (2) (Chapter 2, page 23). Short-wave albedo of the water was estimated following the cyclic monthly pattern proposed by Gallego-Elvira et al. (2010) in a 5m-deep water body for the studied area.

The daily evaporation rate, E (mm d^{-1}) was derived from the knowledge of T_s by applying a mass transfer equation (Singh and Xu 1997):

$$E = h_v(e_s^* - e_a) \quad (67)$$

Where e_s^* (kPa) is the saturated water vapour pressure for saltwater at the temperature T_w , e_a (kPa) is the actual vapour pressure of the air at 2 m, and h_v refers to the daily-average convective coefficient for water vapour transfer in $\text{mm d}^{-1} \text{ kPa}^{-1}$. h_v was considered to be proportional to the wind speed at 2 m, U (m s^{-1}), and dependent on the area of the water body, A (m^2), through an empirical function $f(A)$, i.e. $h_v = U f(A)$. Different formulations of $f(A)$ can be found in the literature; we applied the function proposed by Martínez-Alvarez et al. (2007) for the study area:

$$f(A) = 0.037 \cdot \log_{10}^2 A - 0.578 \cdot \log_{10} A + 3.583 \quad (68)$$

The influence of water salinity in the saturated vapour pressure for saltwater, e_s^* , was calculated by introducing the relationship between water molar fraction, X_{H_2O} , and water salinity, S , proposed for seawater (NaCl salt solutions) by Kokya and Kokya (2008):

$$X_{H_2O} = 1 - 5.71 \cdot 10^{-4} S \quad (69)$$

where S is in PSU. Then X_{H_2O} was applied to the saturated vapour pressure above pure liquid water, e_s (Richards 1971):

$$e_s^* = X_{H_2O} e_s \quad (70)$$

H_s was calculated as follows:

$$H_s = h_c (T_a - T_w) \quad (71)$$

where h_c is the daily-average coefficient of convective heat exchange ($\text{MJ m}^{-2} \text{K}^{-1} \text{d}^{-1}$). Assuming an analogy between mass and energy transfer, the value of h_c was considered equal to $h_c = \gamma \cdot h_v$, where γ is the psychometric constant (kPa K^{-1}).

To determine Q_{Med} the following equation was applied:

$$Q_{Med} = \frac{c_w V_{in,Med} (T_w - T_{w,Med})}{A} \quad (72)$$

where c_w ($\text{MJ m}^{-3} \text{K}^{-1}$) is the volumetric heat capacity of water at the temperature T_w , $V_{in,Med}$ ($\text{m}^3 \text{d}^{-1}$) is the incoming water from the Mediterranean Sea, and $T_{w,Med}$ stands for the mean daily temperature of the Mediterranean Sea (remote sensing data). The daily value of $V_{in,Med}$ was calculated by solving the daily water balance of the Mar Menor, assuming a constant water level:

$$\frac{\Delta V}{\Delta t} = V_{in} - V_{out} = 0 \quad (73)$$

$$V_{in} = V_P + V_R + V_{in,Med} \quad (74)$$

$$V_{out} = V_E + V_{out,Med} \quad (75)$$

where V is the volume of the lagoon (m^3), Δt is the period of time over which the balance is calculated (1 day) and V_{in} and V_{out} are the inflow and outflow discharges respectively ($\text{m}^3 \text{ d}^{-1}$). The inflow discharges are precipitation, V_p , runoff and groundwater discharges, V_R , and incoming water from the sea during the high tides, $V_{\text{in,Med}}$. The outflow discharges are evaporation, V_E , and the outgoing water to the sea during the low tide, $V_{\text{out,Med}}$. The latter was considered a function of wind speed. Direct runoff inflow was disregarded in the study (see Chapter 3, page 68).

The energy stored (or lost) by the lagoon, ΔQ_w , was computed through the following equation:

$$\Delta Q_w = c_w D \frac{\Delta T_w}{\Delta t} \quad (76)$$

where D (m) stands for the mean depth of the water body and $\Delta T_w / \Delta t$ is the variation of water temperature occurring during the daily time step.

6.4.2. Results and discussion

❖ Water temperature in Mar Menor

The outputs provided by the model are the lagoon evaporation and water temperature and water exchanged with the Mediterranean Sea. The model validation was carried out by comparing the simulated daily T_w values with those derived from MODIS-SST images. This validation approach was considered due to the lack of direct measurements of evaporation in Mar Menor, such as water height data (water level variations as a result of water inputs and outputs are minimal) or eddy correlation technique data. Figure 61 shows the agreement between the predicted and the remotely sensed T_w for 2003, 2004 and 2005.

Figure 61: Comparison of the predicted water temperature (T_w model) and the obtained using remote sensing (T_w satellite) in the Mar Menor during the years a) 2003, b) 2004 and c) 2005.

During the late spring and summer, a slight overestimation of the predicted T_w was detected, which varies between +0.5 and +1.5 °C with respect to the remotely sensed values, and this overestimation disappears in subsequent autumn days. During the rest of the year, the differences between the predicted and the remotely sensed T_w ranged between -1 and +1 °C, without any clear trend. Figure 62 shows the regression analysis of the predicted and the remotely sensed daily values of T_w for the study period.

Figure 62: Regression analysis between the predicted and the remote sensed water temperature (T_w) for the period 2003-2006.

A very high correlation can be observed ($R^2 = 0.988$), although the slope is a little lower than 1 (0.940) and the intersection with the ordinate axis is close to 1 °C (0.835 °C). If the intersection is forced to zero, the slope increases to 0.974. These results again indicate that the model slightly overestimates T_w with respect to remotely sensed T_w under high temperature water conditions, whereas the model marginally underestimates under low temperature conditions. The root mean square error (RMSE) between the daily modelled and measured T_w was 0.933 °C, and measures both systematic and random errors whereas the mean bias error (MBE) was 0.551 °C, and measures systematic errors. The low RMSE indicates a fairly good performance of the model, whereas the positive value of MBE makes clear the model's tendency to overestimate T_w as explained above.

This difference could be ascribed to the lack of precision of the values of T_w retrieved from remote sensing, whose accuracy was around ± 0.4 °C (Reinart and Reinhold 2008), and to the model's performance. However, the characteristic overestimation of T_w

during the late spring and summer (+0.5 and +1.5 °C) does not seem to be related to a model inaccuracy. A possible explanation for this could be that the cooling of Mar Menor's surface during midday affects the values of T_w derived from MODIS-SST images (captured from 12:30 to 14:00 GMT). In agreement with this suggestion, several studies (Mas 1996; Rosique 2000) have pointed out a slight and sporadic vertical thermal gradient (2 - 3°C) during summer daytime. Therefore, the hypothesis of an isothermal behaviour of Mar Menor was adequate for modelling purposes, but it produced a minor error when validating the model with remotely sensed data.

❖ Mar Menor's energy balance components

Table 22 displays the monthly and annual average and standard deviation of the energy balance components (Eq. 66) for the study period, calculated from the modelled daily values. Figure 63 presents the predicted daily values of the heat balance components for Mar Menor during the year 2003.

Table 22: Monthly and annual average and standard deviation of the heat balance components during the period 2003 to 2006. The components are net radiation (R_n), sensible heat (H_s), heat exchange with the Mediterranean Sea (Q_{Med}), evaporation flux (λE) and variation of heat in the lagoon (ΔQ_w).

	R_n W m ⁻²	SD W m ⁻²	H_s W m ⁻²	SD W m ⁻²	Q_{Med} W m ⁻²	SD W m ⁻²	λE W m ⁻²	SD W m ⁻²	ΔQ_w W m ⁻²	SD W m ⁻²
Jan	34.2	5.5	-5.8	5.6	2.09	0.34	-36.7	8.3	-6.2	11.6
Feb	61.3	3.5	-9.1	4.3	1.33	0.58	-40.7	6.4	12.8	11.1
Mar	113.5	11.3	-11.9	8.9	-0.56	0.50	-61.6	10.6	39.4	20.0
Apr	161.5	10.5	-28.4	0.8	-2.71	0.91	-104.3	15.0	26.0	8.0
May	190.9	15.4	-34.4	5.3	-4.15	0.73	-133.2	20.3	19.1	12.9
Jun	220.7	7.3	-28.9	5.7	-4.51	1.04	-157.0	10.9	35.2	9.6
Jul	221.0	2.6	-30.2	2.8	-4.40	0.67	-175.6	7.9	10.1	9.5
Aug	191.7	6.6	-25.5	2.6	-3.20	0.32	-175.8	12.5	-12.8	9.3
Sep	136.2	6.3	-22.3	3.3	-1.76	0.49	-134.0	7.8	-21.9	5.6
Oct	77.8	6.5	-19.3	2.2	-0.45	0.40	-92.6	11.5	-34.5	14.2
Nov	30.4	3.9	-15.2	2.3	1.32	0.36	-60.6	13.2	-44.1	18.8
Dec	20.3	2.6	-5.3	5.9	2.39	0.26	-43.8	4.6	-26.4	12.6
Annual	122.0	2.0	-19.7	1.2	-1.22	0.21	-101.3	1.6	-0.3	0.8

Net radiation (R_n) presented the largest values in July and the lowest in December. The monthly R_n value was positive during the whole year, but the daily R_n presented some negative values during the wintertime (Figure 63) on days with very cloudy conditions. Furthermore, the ratio $r = R_n/R_s$ was 0.58 on an annual basis, with strong differences between July ($r \approx 0.70$) and December ($r \approx 0.20$).

At a daily scale, a high temporal variability of the evaporation was observed, mainly associated with the great variability of the wind regimes in the area due to the sea exposure. λE displayed a few positive daily values in late winter and early spring (Figure 63) when air temperature increases more rapidly than the lagoon surface temperature due to the large heat capacity of the lagoon. During these days, condensation predominated over evaporation and λE flux could be considered as a fresh water input. Maximum daily values were observed in summer, when λE surpassed 284 W m^{-2} in several occasions.

Monthly latent energy flux (λE) was the more important heat loss, accounting for 82.9% of the annual losses. Monthly λE flux increased rapidly from February to July, reaching its highest values in August (175.8 W m^{-2}), followed by a rapid decline in autumn and reaching low steady rates ($\approx 40 \text{ W m}^{-2}$) in winter. A time lag of two months with regard to the maximum and minimum values of R_s was observed due to the high thermal inertia of the water body. The annual λE ranged between 99.77 and 103.63 W m^{-2} , with the mean value of the studied period being 101.3 W m^{-2} (equivalent to $1,310 \text{ mm y}^{-1}$). For the same period, the annual Class-A pan evaporation rate in the Mar Menor area varied from $1,700$ to $1,800 \text{ mm y}^{-1}$ (Martínez Alvarez et al. 2008). For these values, the pan coefficient (ratio between the water body and Class-A pan evaporation rates) ranges from 0.696 to 0.736 , values similar to the ones recommended in the literature for large water bodies (Linacre 1994). The annual reference evapotranspiration estimated using the Penman-Monteith method is also considered by many authors to be a valid reference to estimate the annual E in water bodies. Its mean annual value for the studied period at the meteorological station of the San Javier airport is $1,344 \text{ mm y}^{-1}$, very close to the value estimated by the model. All these values corroborate the validity of evaporation estimations provided by the model.

Sensible heat (H_s) was relatively small compared to the other components. The annual average H_s was -19.7 W m^{-2} , accounting for 16.1% of the annual heat losses. Daily H_s values (Figure 63) showed that during the spring, summer and autumn the lagoon usually loses sensible heat because the lagoon's temperature is higher than the air temperature. Conversely, during wintertime, positive values of H_s are frequent and the lagoon takes heat from the atmosphere.

Figure 63: Daily heat balance (Eq.1) in the Mar Menor for the year 2003. See legend in Table 22.

The energy exchange with the Mediterranean Sea (Q_{Med}) was very small compared to the rest of the heat balance components, amounting to only 1% of the annual losses. Only a slight heat loss was observed from March to October, when $T_{Med} < T_w$, and a small heat gain was observed during the rest of the year, when $T_{Med} > T_w$.

Lastly, the heat storage (ΔQ_w) showed a high daily variability (Figure 63) that is balanced between positive and negative values on an annual basis. The evolution of monthly ΔQ_w was characterized by an annual cycle with a 6-month period of heat storage (from February until July) followed by another 6-month period of heat release (from August to January). This fact explains the two-months lag phase between the time of occurrence of the maximum and minimum fluxes of R_n and λE . In the warm season, the downwelling solar radiation is absorbed throughout the water column, rather than at the surface, as is the case with other land surfaces. This heat is afterwards released during the fall, enhancing the evaporation and decoupling this term from net radiation.

The monthly trend of the Bowen ratio, $B = H_s/\lambda E$, was calculated using the estimates of λE and H_s (Table 22). Monthly B was rather conservative throughout the year, varying within the range of 0.10 – 0.30. Daily B showed a very small variability during the warm season, while a large variability was observed for the winter months. This was due to the occurrence of negative values of B corresponding to very cloudy conditions and low available energy. The magnitude of the annual value of B ($= 0.194$) was similar to previously published estimations for large water bodies under different climate conditions, for example, 0.23 for Sparkling Lake in USA (0.64 km², mean depth 10.9 m, Lenters et al. 2005), 0.21 for Lake Titicaca in South America (8,560 km², mean depth 105 m, Delclaux et al. 2007) and 0.19 for Lake Ikeda in Japan (10.62 km², mean depth 125m, Momii and Ito 2008).

6.5. Conclusion

This Chapter pretended to put into practice the potential of remote sensing techniques to retrieve spatio-temporal estimation of surface fluxes through three operational applications. The first one illustrates how the RS-based triangle method can generate ET-maps that assist the spatio-temporal characterisation of surface fluxes in regions of interest in Western Africa. In particular, the effect of the West-African monsoon on the energy fluxes can be clearly identified and a clear moisture-control over ET could be determined. The monsoon has a different degree of impact for the three studied sites, as a clear North-South gradient of precipitation can be observed.

The second operational tool presented in this Chapter is the use of the same RS-based method to characterise the annual behaviour of SEB components at three sites of interest in South-East Spain, over a 12-year time series. This exercise allows delineating a RS-based SEB components climatology in the studied area. Our analysis reveals different annual trends of ET and EF at the three sites, with maximum in summer for the irrigated sites (Murcia and Calasparra), and maximum in the fall season for the driest site (Jumilla) which corresponds to the period with the highest probability of rainfall in the Segura River Basin. The annual amplitude differs among sites, indicating the effect of the significantly lower annual rainfall at the driest site (Jumilla), or an effect of intensively irrigated agriculture at the Murcia site eventually coupled to local advection effects during the warm season.

The third application presented is the use of a mathematical model to characterise the surface fluxes of the coastal lagoon Mar Menor in South-East Spain. The proposed model is used to analyse the daily environmental behaviour of the Mar Menor coastal lagoon during a 4-year period. The model's performance is assessed by comparing the predicted daily water temperatures with those from remotely sensed thermal imagery (MODIS-SST product). A reasonable agreement is obtained between the predicted and the remotely sensed water temperature, which suggests a satisfying performance of the model for retrieving energy fluxes, which are directly dependant on water temperature. The implementation of the techniques used in this study is straightforward and relatively cost effective, and the data needed are standard and readily available, which makes its operational use simple and attractive.

Chapter 7: Conclusions

7.1. Synthesis of the results

A relevant contribution of our study is the proposal of a new parameterisation scheme of ground heat flux (G) for retrieving surface fluxes from remote sensing data (MODIS-Terra). Formulae that are based on empirical relationships relating G to net radiation, R_n ($G = \alpha R_n$, α being a function of a vegetation index, VI) are currently used, but presented drawbacks, especially in bare or sparse vegetation areas because of the poor adequacy of VI-based relationships to account for changes in soil moisture. In this study, we proposed to link α to the evaporative fraction, EF. In a first step, using a non-dimensional form of the surface energy balance, we demonstrated that α is functionally related to EF and to the ratio $\gamma = G/H$ (H = sensible heat flux). In a second step, we proposed an EF-based parameterisation of α , using ground fluxes data sets collected throughout the years 2005, 2006 and 2007 at four flux-tower sites in West African countries (Mali, Benin, Niger) that differ in surface conditions and Monsoon influence. The analysis indicated that the average site-specific values of α and EF were well described by a linear relationship of the type $\alpha = a \text{ EF} + b$, with $a = -0.22$ and $b = 0.23$. In a third stage, we investigated whether ET-retrieval algorithms remote sensing information (MODIS-Terra) using the new parameterisation of α perform better than the classical formulation through VI-based relationships. We found that the retrieved values of H using the new parameterisation supplied the best agreement with the observed ground data and significant improvement with respect to estimates from α -VI relationships. The main advantage of the new parameterisation of G is that it implicitly accounts for changes in soil moisture status through EF, delivering more realistic estimations than the traditional VI-based parameterisations. One of the main limitations was that the scheme is only valid at the satellite overpass time due to the time lag existing between G and H . This was partially overcome, for the dry season, by the combination of the new scheme with the formulation proposed by Santanello and Friedl (2003) to estimate α at different time of the day.

The other original contribution derives from the comparative analysis between the RS-based triangle method and the JULES land surface model. A preliminary analysis using the default-run version revealed an overestimation of the surface conductance that

controls evapotranspiration process within JULES, resulting in substantial differences in ET-JULES with respect to ET-triangle in spring and summer. The disagreement between JULES and the triangle estimations was ascribed to inadequate values of the input parameters in the JULES default-run version. In a second step, a sensitivity analysis of JULES to a series of input parameters was carried out using the Monte Carlo (MC) method. It was found that soil properties parameters produced the largest uncertainties on ET, especially soil albedo, soil moisture at the critical point and soil moisture at wilting point. In a third step, the MC method was assessed as a calibration tool using RS-based estimations of ET to adjust the input parameters. When calibrated in that way, the performance of JULES was highly improved, and could reproduce ET-trends observed with the RS-based algorithm. However, some of the adjusted parameters presented unrealistic values, suggesting that the improved model performance is probably the result of some mathematical artefact. We therefore recommend caution when applying the MC-method for LSM parameterisation.

The last part of the thesis presents some potential applications of the above operational tools. The first application presented was the use of the RS-based triangle method to retrieve ET-maps in Western Africa. The spatiotemporal characterisation of surface fluxes allowed identifying and quantifying the effects of the West-African monsoon, with a clear South-North gradient.

The second application was the analysis of a 12-year series (2000-2011) of LST, EF and ET estimates by the Triangle algorithm using MODIS-LST and VI observations. We presented monthly and inter-annual of EF and ET variations at three sites of the Segura River Basin and combined these measurements with ground meteorological data (T_a , VPD_a) in an intent to disentangle the physical mechanisms implicated in mean-to-long term changes of surface fluxes variations and their control by natural and/or human-induced actions. Notwithstanding the uncertainties and errors associated with RS information and ET-retrieval methods, this attempt to build a climatology of RS-observed (e.g. LST) or RS-retrieved (e.g. EF) land surface attributes is encouraging. In particular, the results presented in form of average year appear coherent, enabling to describe and quantify the impact of the main drivers (rainfall, irrigation, type of surface and land use) that determine the annual trend of variables such as EF, of paramount importance for assessing the hydrological balance and the impact of climate and land use on water resources.

The third application was the use of sea surface temperature observations to validate a water balance model of a coastal lagoon (Mar Menor) in South-East Spain. Once

the model was validated with the RS-data, the outputs agreed satisfactorily with the observations. The proposed model was then used to analyse the thermal behaviour of the Mar Menor coastal lagoon during a 4-year period.

7.2.Implications of the PhD work for future research and applications

The new parameterisation represents a progress and improvement in the representation of G for RS-based retrieval of surface fluxes compared to traditional VI-based parameterisation used currently. Further research is necessary to translate this new parameterisation scheme for G to other semi-arid areas of the world and check its universal validity, and to generalise its implementation into operational tools for monitoring SEB components. This would greatly assist and improve current water management systems and environmental monitoring schemes in assessing the real state of water availability and energy balance status in semi-arid regions.

The comparative analysis of JULES with the RS-based triangle method suggests that a tool combining a LSM with a RS-based algorithm to estimate ET could potentially be a solution to get continuous and reliable surface fluxes estimation and to overcome the limitations of each individual method. Future work is needed to improve the way in which the two approaches can be combined. Data assimilation techniques could be the answer to efficiently merge the two methods, although the computational implications and the complexity of the models to be handled could be an obstacle to their operational use.

In a recent paper, van Dijk and Renzullo (2011) point out the current lack of operational water resources monitoring system that integrate RS-based information. Their review of operational and research applications demonstrates the utility of satellite information in improving accuracy and spatial details in monitoring water balance components. They conclude that the future should be a moving towards the integration of RS-based methods and data assimilation techniques within spatial water resource monitoring systems (SWRMS) in order to improve the accuracy and spatial details of existing methods to better support water management decisions.

The results of this PhD are a starting point to answer their concern. SWRMS can provide valuable information in support of water management, but current operational systems are few and provide only a subset of the information required. Necessary innovations include the explicit description of water redistribution and water use from

river and groundwater systems, achieving greater spatial detail (particularly in key features such as irrigated areas, wetlands and water bodies), and improving accuracy as assessed against hydrometric observations, as well as assimilating those observations. There are indications that the development of operational SWRMS is currently progressing rapidly however, particularly now that some of the main technological obstacles have been overcome. Internet communication and telemetry have become fast and inexpensive. Reliable and accessible near-real time satellite data services have become available (though much data is still collected by research missions and therefore arguably not truly operationally reliable). Robust yet flexible information and communications technology (ICT) solutions have been developed to support the development of operational systems. The challenge, therefore, is on the climatological and hydrological community to develop modelling systems that integrate satellite and on-ground observation systems as necessary to produce water resources information that is of use to decision makers.

Operational challenges include the continuity of research satellite missions and data services, and the need to find computationally-efficient data assimilation techniques. The successful use of observations critically depends on the availability of detailed information on observational error and understanding of the relationship between remotely-sensed and model variables, as affected by conceptual discrepancies and spatial and temporal mismatches. In this aspect, our study demonstrates that the adoption of RS-based operational tools is feasible and that such tools could be integrated in SWRMS, or in other types of water resources management systems for monitoring water balance components in water-scarce environments.

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